

## **UNIT -1**

# **CHEMISTRY OF SEMICONDUCTORS**

### **1. Semi conductors**

#### **1.1 Introduction**

Semiconductors are materials that have a conductivity between conductors (generally metals) and non-conductors or insulators (such as ceramics). Semiconductors can be compounds such as gallium arsenide or pure elements, such as germanium or silicon. Semiconductors are employed in the manufacture of various kinds of electronic devices, including diodes, transistors, and integrated circuits. Such devices have found wide application because of their compactness, reliability, power efficiency, and low cost. As discrete components, they have found use in power devices, optical sensors, and light emitters, including solid-state lasers. They have a wide range of current- and voltage-handling capabilities and, more important, lend themselves to integration into complex but readily manufacturable microelectronic circuits.

Examples of Semiconductors:

Gallium arsenide, germanium, and silicon are some of the most commonly used semiconductors. Silicon is used in electronic circuit fabrication and gallium arsenide is used in solar cells, laser diodes, etc.

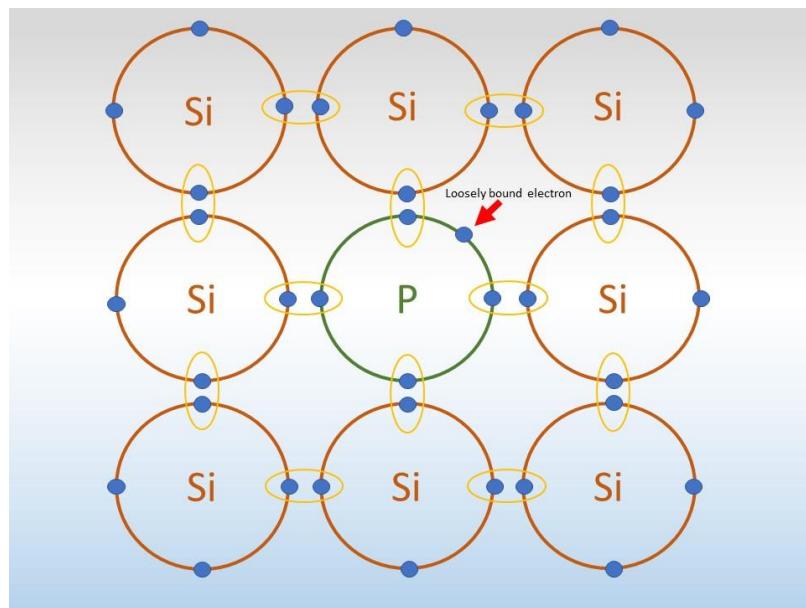
Unlike conductors such as metals, semiconductors are not able to conduct current. This is because they have no free electrons. The most common material used in semiconductors is silicon which only conducts electricity under certain conditions.

#### **1.2. Holes and Electrons:**

Silicon atoms can be stacked to make a crystal. These have regular structures with atoms bound by sharing a pair of electrons. A silicon crystal can't conduct current because the electrons are not free. To change this small amount of energy can be put into the system. This frees the electrons.

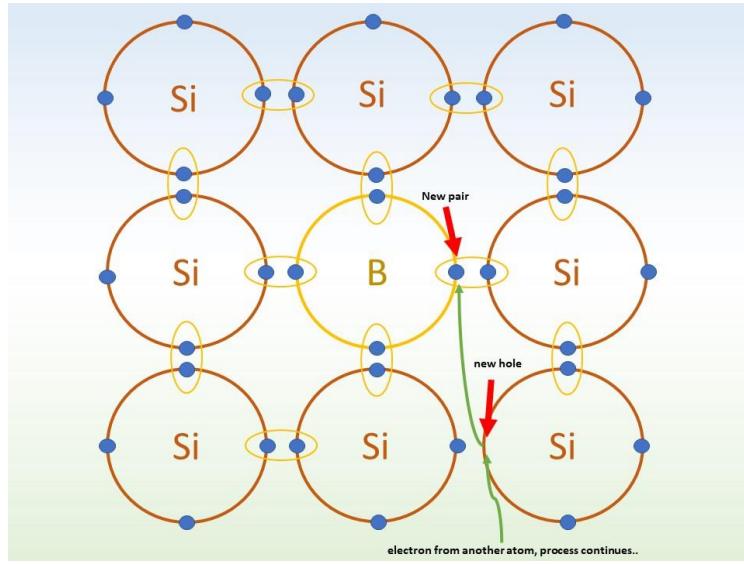
It is possible to make semiconductors better using a process called doping. There are 2 different types of doping. In both cases a different material is added to the crystal. The 2 types are called n-doping and p-doping:

**n-doping:** Here silicon is doped with a material like phosphorus (P). This replaces some silicon atoms in the crystal. The silicon bonds with the phosphorus but leaves behind an extra electron. This is loose inside the crystal and can be freed easily. This lets it conduct electricity. The electrons that are freed have a **negative** charge, so the process is called n-doping.



**Fig 1.1 Holes and Electrons (Si-P)**

**p-doping:** Here the silicon is doped with an atom like boron (B). Like n-doping, the silicon wants to bond four silicon atoms. But boron only has 3 electrons available. The extra electron comes from a neighbor atom. This makes a hole in the parent atom's outer shell. Once this hole is opened, another electron moves to take its place. The hole moves around the crystal! With a **positive** charge this is called p-doping.



**Fig 1.2 Holes and Electrons (Si-B)**

Holes are formed when electrons in atoms move out of the valency band into the conduction band which happens everywhere in semiconductor. The number of holes is always equal to the number of electrons because the appearance of an electron in the conduction band always leads to a hole appearing in the valance band.

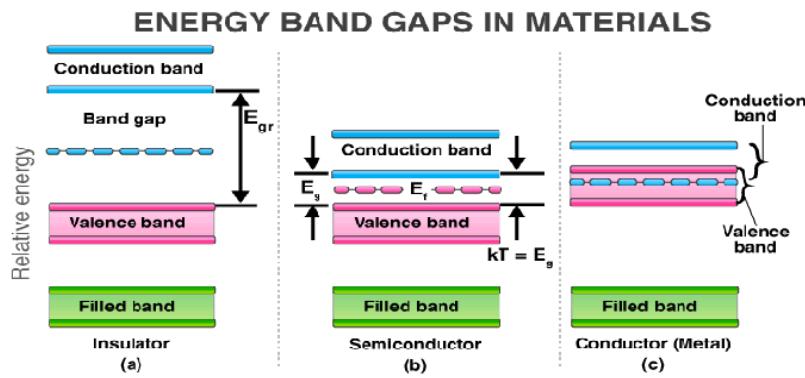
### 1.2.1 Conduction Band and Valence Band in Semiconductors

#### 1.2.1.1 Valence Band:

The energy band involving the energy levels of valence electrons is known as the valence band. It is the highest occupied energy band. When compared with insulators, the band gap in semiconductors is smaller. It allows the electrons in the valence band to jump into the conduction band on receiving any external energy.

#### 1.2.1.2 Conduction Band:

It is the lowest unoccupied band that includes the energy levels of positive (holes) or negative (free electrons) charge carriers. It has conducting electrons resulting in the flow of current. The conduction band possesses high energy level and are generally empty. The conduction band in semiconductors accepts the electrons from the valence band.



**Fig. 1.3 Conduction Band and Valence Band in Semiconductors**

### 1.3 Band Theory of Semiconductors

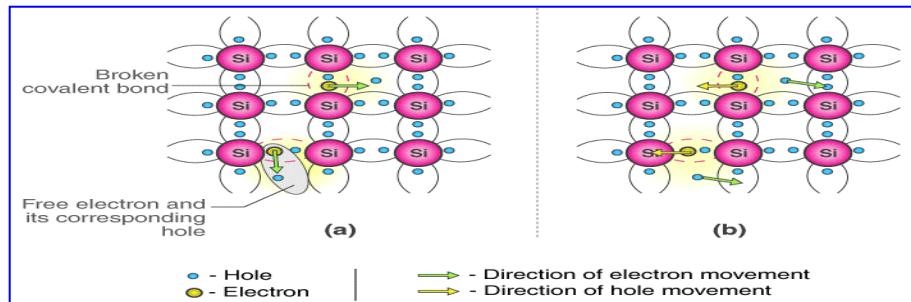
In semiconductors, the conduction band has no electrons. Conduction electrons originate from the thermal excitation of electrons from a lower energy band or from impurity atoms in the crystal (doping).

We know that the electrons in an atom are present in different energy levels. When we try to assemble a lattice of a solid with  $N$  atoms, then each level of an atom must split up into  $N$  levels in the solid. This splitting up of sharp and tightly packed energy levels forms Energy Bands. The gap between adjacent bands representing a range of energies that possess no electron is called a Band Gap.

A very large band gap is indicative of an insulator--since it takes a great deal of energy for the electron to "jump" from the valence band to the conduction band, there will not likely be any conductivity. In conductors (metals) there is zero band gap, therefore the valence and conduction bands overlap. This allows for constant conductivity. Semiconductors thus have a very small band gap, meaning that their conductivity is in between that of an insulator and conductor.

## 1.4 Properties of Semiconductors

1. Semiconductor acts like an insulator at Zero Kelvin. On increasing the temperature, it works as a conductor.
2. Due to their exceptional electrical properties, semiconductors can be modified by doping to make semiconductor devices suitable for energy conversion, switches, and amplifiers.
3. Lesser power losses.
4. Semiconductors are smaller in size and possess less weight. Their resistivity
5. (**Resistivity:**  $10^{-5}$  to  $10^6 \Omega\text{m}$ ) is higher than conductors but lesser than insulators.
6. The resistance of semiconductor materials decreases with the increase in temperature and vice-versa.

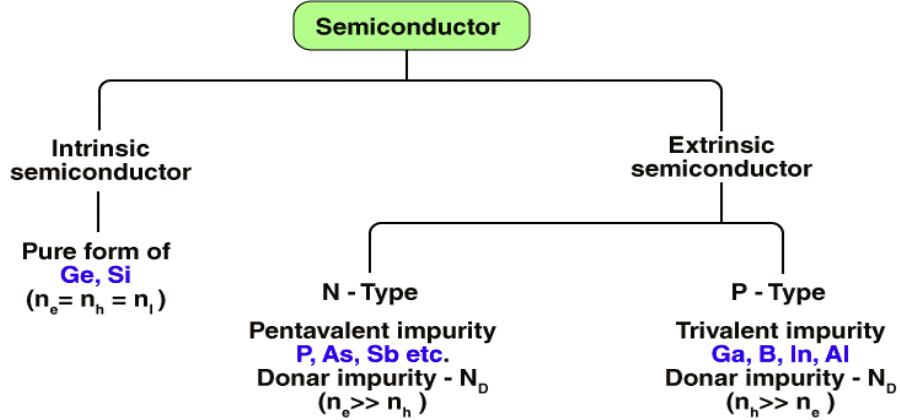


Absence of  
electrical field

Presence of  
electrical field

Fig. 1.4 Properties of Semiconductors

## 1.5 Types of semiconductors:



### 1.5.1 Intrinsic Semiconductor

- Intrinsic semiconductor material is chemically very pure and possesses poor conductivity.
- It has equal numbers of negative carriers (electrons) and positive carriers (holes)

### 1.5.2 Extrinsic Semiconductor

- Extrinsic semiconductor is an improved intrinsic semiconductor with a small amount of impurities added by a process, known as doping, which alters the electrical properties of the semiconductor and improves its conductivity.
- Introducing impurities into the semiconductor materials (doping process) can control their conductivity.
- Doping process produces two groups of semiconductors:
  - The negative charge conductor (*n*-type) and the positive charge conductor (*p*-type)
- Semiconductors are available as either elements or compounds.
- Silicon and Germanium are the most common elemental semiconductors.

Compound Semiconductors include InSb, InAs, GaP, GaSb, GaAs, SiC, and GaN

## 1.6 Mobility of Electrons and Holes

In a semiconductor, the mobility of electrons is higher than that of the holes. It is mainly because of their different band structures and scattering mechanisms.

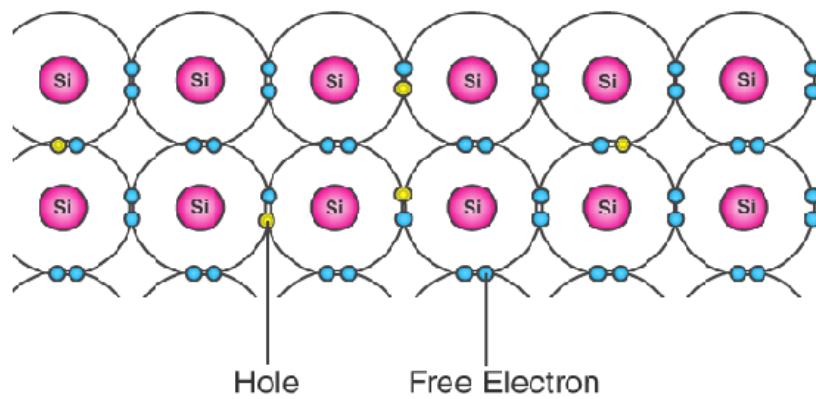
Electrons travel in the conduction band whereas holes travel in the valence band. When an electric field is applied, holes cannot move as freely as electrons due to their restricted movement. The elevation of electrons from their inner shells to higher shells results in the creation of holes in semiconductors. Since the holes experience stronger atomic force by the nucleus than electrons, holes have lower mobility.

The mobility of a particle in a semiconductor is more if;

- Effective mass of particles is lesser
- Time between scattering events is more

For intrinsic silicon at 300 K, the mobility of electrons is  $1500 \text{ cm}^2 (\text{V}\cdot\text{s})^{-1}$  and the mobility of holes is  $475 \text{ cm}^2 (\text{V}\cdot\text{s})^{-1}$ .

The bond model of electrons in silicon of valence 4 is shown below. Here, when one of the free electrons (blue dots) leaves the lattice position, it creates a hole (yellow dots). This hole thus created takes the opposite charge of the electron and can be imagined as positive charge carriers moving in the lattice.



**Fig. 1.5 Mobility of Electrons and Holes**

### **1.7 Fermi level in Semiconductors:**

Fermi level is present between the valence and conduction bands. It is the highest occupied molecular orbital at absolute zero. The charge carriers in this state have their own quantum states and generally do not interact with each other. When the temperature rises above absolute zero, these charge carriers will begin to occupy states above Fermi level.

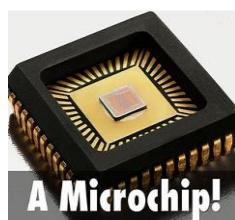
In a p-type semiconductor, there is an increase in the density of unfilled states. Thus, accommodating more electrons at the lower energy levels. However, in an **n-type** semiconductor, the density of states increases, therefore, accommodating more electrons at higher energy levels.

### **1.8 Industrial Applications of Semiconductors:**

- The physical and chemical properties of semiconductors make them capable of designing technological wonders like microchips, transistors, LEDs, solar cells, etc.

#### **1. Microchip**

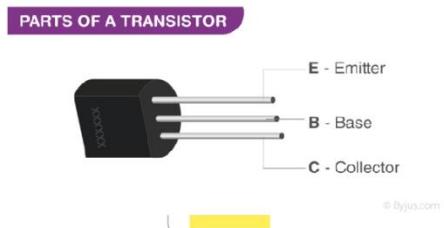
A microchip (also called a chip, a computer chip, an integrated circuit or IC) is a set of electronic circuits on a small flat piece of silicon. The good news is that it's everywhere! Silicon is made from sand, and it is the second most abundant element on earth after oxygen. Silicon wafers are made using a type of sand called silica sand, which is made of silicon dioxide. The sand is melted and casted in the form of a large cylinder called an 'ingot'. This ingot is then sliced into thin wafers. A microchip the size of your fingernail contains billions of transistors, so it's easy to understand just how small the features on a chip need to be. Chip features are measured in nanometers.



**Fig 1.6 Microchip**

## 2. Transistor

A transistor is an electronic component, a semiconductor device with three connections, that is used in circuits to either amplify or switch electrical signals or power, allowing it to be used in a wide array of electronic devices.



**Fig 1.7. Transistor**

## 3. Microprocessor

A Microprocessor is an important part of a computer architecture without which one will not be able to perform anything on his computer. It is a programmable device that takes in input performs some arithmetic and logical operations over it and produces the desired output. In simple words, a Microprocessor is a digital device on a chip that can fetch instructions from memory, decode and execute them and give results. The microprocessor used for controlling the operation of space vehicles, trains, robots, etc is made up of transistors and other controlling devices which are manufactured by semiconductor materials.

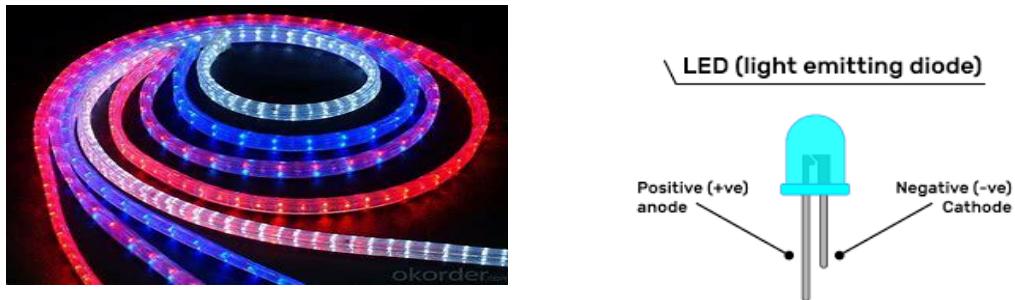


**Fig 1.8. Microprocessor**

## **1.9 Semiconductors in Optics:**

### **1.9.1 LEDs:**

A light-emitting diode (LED) is a semiconductor device that emits visible light when an electric current passes through it. The light is not particularly bright, but most LEDs it is monochromatic, occurring at a single wavelength.



**Fig 1.9. Light Emitting diodes**

#### **1.9.1.1 Features:**

1. Transparent PVC housing for waterproof.
2. Unique structure, more energy saving, environmental protection, long life.
3. Can be cut to size at marked intervals and rejoined by electricians.
4. Solid-state for high vibration resistance and good flexibility for any shape.
5. Operating temperature: -20°C~+60°C
6. Color temperature: Cool white 6000-6500K and warm white 2700-3200K
7. Available color: red, yellow, blue, green, white, orange, pink, purple, multicolor and RGB.
8. Solid, hollow is available
9. Working current: 15-18ma

#### **1.9.1.2 Applications:**

- 1) Architectural decorative lighting
- 2) Archway, canopy and bridge edge lighting

- 3) Amusement park, theater and aircraft cabin mood lighting
- 4) Emergency hallway lighting
- 5) Auditorium walkway lighting
- 6) Stairway accent lighting
- 7) Concealed lighting
- 8) Backlighting for signage letters
- 9) Channel letter lighting
- 10) Emergency exit path lighting
- 11) Cove lighting

### **1.9.2 OLEDs**

Organic light emitting diodes (OLEDs) are comprised of a thin layer of light emitting organic material sandwiched between two electrical contacts

#### Working

- An electrical current flows from the cathode to the anode through the organic layers.  
The cathode gives electrons to the emissive layer of organic molecules.
- The anode removes electrons from the conductive layer of organic molecules.
- At the boundary between the emissive and the conductive layers, electrons find electron holes.
- When an electron finds an electron hole, the electron fills the hole.
- When this happens, the electron gives up energy in the form of a photon of light
- The OLED emits light.
- The color of the light depends on the type of organic molecule in the emissive layer.  
Manufacturers place several types of organic films on the same OLED to make color displays.
- The intensity or brightness of the light depends on the amount of electrical current applied: the more current, the brighter the light.

## Organic Light-emitting Diode

**Cathode** is an electrode that allows electric current to flow through

**Emissive Layer** is a color filter of pixels made up of Polymers

**Conductive Layer** is design to transport electrons

**Anode** removes electrons from the Conductive layer

**Substrate** is the plastic film of the OLED

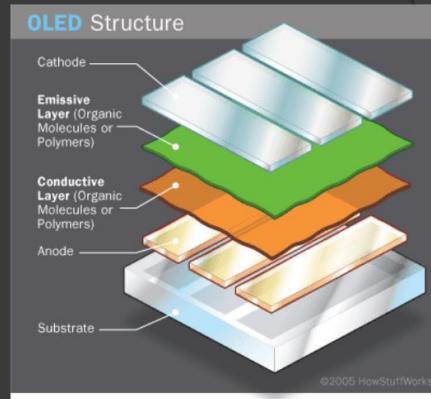


Fig 1.10 Organic Light- Emitting diodes

### 1.9.2.1 Uses:

Used in Flat Screen Monitors, Flat Screen TVs, Military Use



Fig. 1.11 OLED TV

## **1.10 Semiconductors in Solar cells:**

A solar cell, or photovoltaic cell, is an electronic device that converts the energy of light directly into electricity by the photovoltaic effect, which is a physical and chemical phenomenon.

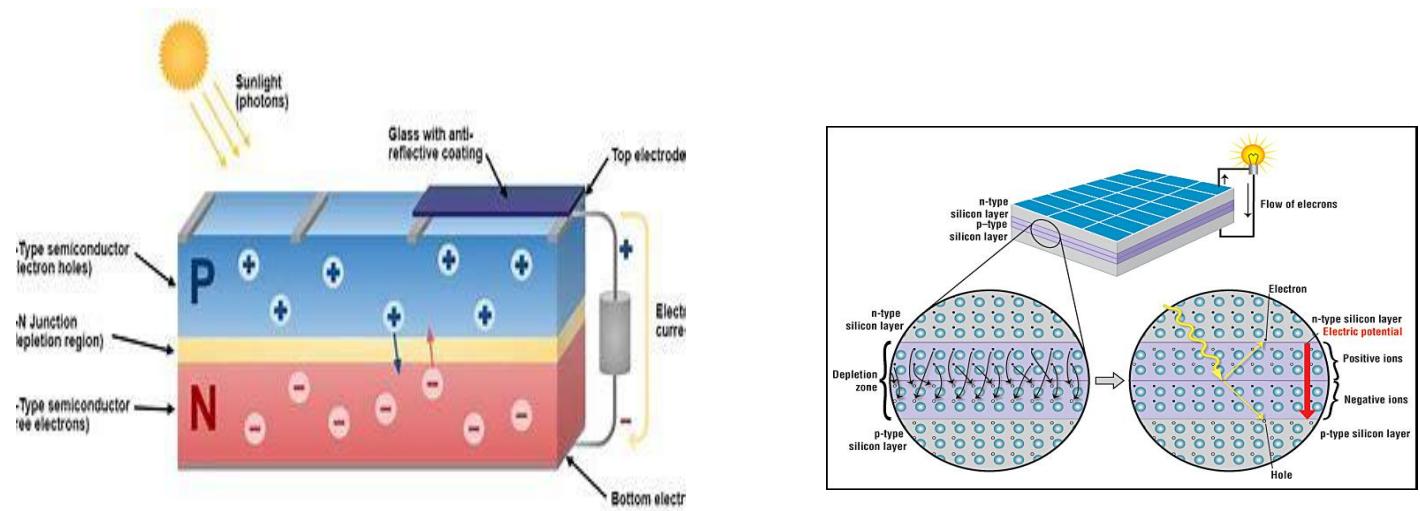
A solar cell is made of two types of semiconductors, called p-type and n-type silicon. The p-type silicon is produced by adding atoms such as boron or gallium that have one less electron in their outer energy level than does silicon. Because boron has one less electron than is required to form the bonds with the surrounding silicon atoms, an electron vacancy or “hole” is created.

The n-type silicon is made by including atoms that have one more electron in their outer level than does silicon, such as phosphorus. Phosphorus has five electrons in its outer energy level, not four. It bonds with its silicon neighbor atoms, but one electron is not involved in bonding. Instead, it is free to move inside the silicon structure.

A solar cell consists of a layer of p-type silicon placed next to a layer of n-type silicon. In the n-type layer, there is an excess of electrons, and in the p-type layer, there is an excess of positively charged holes (which are vacancies due to the lack of valence electrons). Near the junction of the two layers, the electrons on one side of the junction (n-type layer) move into the holes on the other side of the junction (p-type layer). This creates an area around the junction, called the depletion zone, in which the electrons fill the holes. When all the holes are filled with electrons in the depletion zone, the p-type side of the depletion zone (where holes were initially present) now contains negatively charged ions, and the n-type side of the depletion zone (where electrons were present) now contains positively charged ions. The presence of these oppositely charged ions creates an internal electric field that prevents electrons in the n-type layer to fill holes in the p-type layer.

When sunlight strikes a solar cell, electrons in the silicon are ejected, which results in the formation of “holes”—the vacancies left behind by the escaping electrons. If this happens in the electric field, the field will move electrons to the n-type layer and holes to the p-type layer. If you connect the n-type and p-type layers with a metallic wire, the electrons will travel from the

n-type layer to the p-type layer by crossing the depletion zone and then go through the external wire back of the n-type layer, creating a flow of electricity.



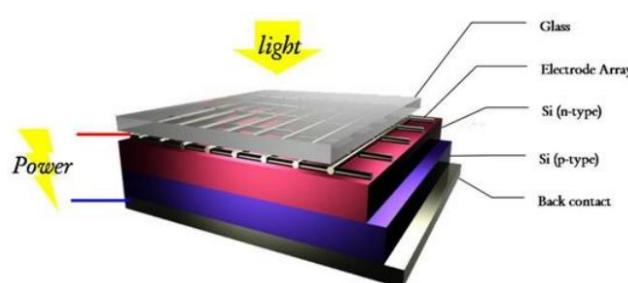
**Fig.1.12 Semiconductors in Solar cells**

## 1.11 Types of Solar Cells

### 1.11.1 First-Generation Solar Cells:

First generation solar cells are made of crystalline silicon, also called, conventional, traditional, wafer-based solar cells and include monocrystalline (mono-Si) and polycrystalline (multi-Si) semiconducting materials

Example: Silicon Wafers



**Fig.1.12 Semiconductors in Solar cells**

About 90 percent of the world's solar cells are made from wafers of crystalline silicon (abbreviated c-Si), sliced from large siliconingots(a cylindrical mass) into disk-shaped pieces of about 0.5mm to 1mm thick, which are grown in super-clean laboratories in a process that can take up to a month to complete. The ingots either take the form of single crystals (monocrystalline or mono-Si) or contain multiple crystals (polycrystalline, multi-Si or poly c-Si).

There are various methods used in silicon fabrication counting the horizontal Bridgeman method, horizontal gradient freeze method, vertical gradient freeze, vertical Bridgeman method and the Czochralski pulling method.

### **1.11.2 Single Crystalline and Poly crystalline Solar Cells:**

Silicon which is the key raw material in crystalline silicon solar photovoltaic is extensively available in the form of silica (silicon dioxide) on and in the earth's crust. But both monocrystalline and polycrystalline silicon solar cells require ultra-pure silicon which is not available in nature.

So, silicon must be extracted from silica and then needs to be purified up to solar grade silicon. Silicon is extracted from sand or quartz by heating with a reducing agent which is usually high purity coke or coal. In this process, an excessive amount of silica is used to reduce the formation of silicon carbide. During the process, oxygen combines with carbon to produce carbon dioxide and escape from the furnace leaving molten silicon. Extracted silicon in this reaction is, about 99% pure which is, however, not pure enough for the fabrication of solar cells. It needs to be purified further to obtain solar grade silicon.

The purity of 2N silicon material cannot be used directly to prepare solar cells, so further purification is required. In history, people have proposed many purification methods for silicon materials, but the Siemens method is currently the most commonly used in the industry. The basic idea of the Siemens law is: firstly, low-purity silicon is hydrogenated to prepare trichlorosilane ( $\text{SiHCl}_3$ ) gas, and then  $\text{SiHCl}_3$  is purified by distillation. The high-purity  $\text{SiHCl}_3$  is sent to a reduction furnace to be reduced to high-purity silicon.

The next step is to obtain cylindrical ingots of high purity silicon. While several methods are available to grow single crystalline silicon, Czochralski process is widely used due to its intrinsic advantages over other techniques.

As its name implies, Mono crystalline silicon is made of a single crystal. The entire sample is made of an unbroken, high purity single crystal of silicon. Hence, single crystalline silicon contains no grains or grain boundaries.

A polycrystalline solid or polycrystal is comprised of many individual grains or crystallites. Each grain can be thought of as a single crystal, within which the atomic structure has long-range order.

## **1.12 Czochralski (CZ) method**

### **1.12.1 Terminology**

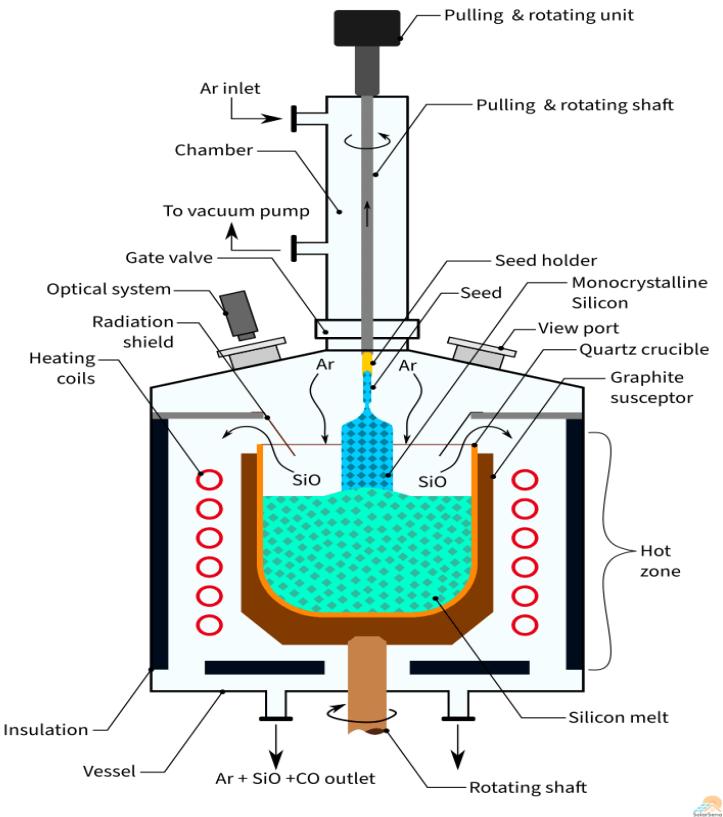
1. Crystal growth: It is an important process in crystallization in which newer structures unite in a specific pattern to form a crystal.
2. Monocrystal: It is a crystal having unbroken crystal lattice throughout the material. Monocrystals have no grain boundaries and are free from defects. Other terms for it are single crystal and monocrystalline.
3. Ingot: Ingot is a pure piece of material.
4. Seed: A seed crystal is a tiny piece used to grow a larger crystal. It promotes the growth rate when brought in contact with the solution.
5. Dopant: Dopants are foreign substances added to magnify the electrical properties of semiconductors.

### **1.12.2 Schematic Representation of Czochralski process**

The diagram below represents a simple industrial schematic of the Czochralski process. The description of the main elements in the diagram is as follows:

1. Quartz crucible: A crucible made of quartz is a container in which silicon is melted. Quartz is a mineral and consists of  $\text{SiO}_2$ . It has a melting point above 1650 °C.
2. Melt: The melt is liquid silicon in the crucible.

3. Heating coils: Heating coils are an induction heater used to heat silicon in the crucible. They generate heat by Joule heating i.e., when a high current flow through a conductor, the resistance of the conductor produces heat.
4. Pulling and rotating shaft: The pulling and rotating shaft is a rotating rod or wire used to lift the cylindrical monocrystalline silicon. In the figure, it is rotating anticlockwise.
5. Crucible shaft: Another rotating shaft, it is affixed to the crucible. Its direction of rotation can be the reverse or the same as the pulling & rotating shaft. In the figure, it is rotating clockwise.
6. Insulation: Insulation prevents heat from escaping the vessel.
7. Radiation shield: Temperatures in the vessel are very high. To minimize energy losses and to avoid exposure to radiation, the radiation shield is used.



**Fig.1.13 Czochralski process**

### **1.12.3 Working of Czochralski process**

Crushed high-quality polycrystals of silicon are placed in a quartz crucible. Dopant impurities, like boron, phosphorus, are also mixed with polycrystals in the right proportion. Boron will create p-type silicon; phosphorus will create n-type silicon.

The heat required to melt the materials is provided by induction coils. As the temperature of the system increases, polycrystals will start melting. The melting point of polycrystalline silicon is around 1414 °C. To have complete melting, we keep the temperatures inside the vessel slightly higher than the melting point, around 1420 to 1425 °C. Keeping high temperatures for a while removes any tiny bubbles present in the melt. It decreases the chances of defects during crystallization.

#### **1.12.3.1 Seeding**

A seed with a known crystal orientation is lowered and partially dipped in the melt. The vertical motion of the seed is controlled by the shaft.

As the seed starts to melt, it is slowly pulled upward and at the same time rotated. The rotation of the seed and crucible increases homogeneity.

When the seed is lifted upward, it carries a small portion of the molten liquid with it due to surface tension. It causes cooling and crystallization of the liquid portion near to the seed.

By regulating the temperature profile and pulling rate, the diameter of the crystal is gradually increased. In the process, the conical region, or shoulder, are formed.

## **SELF ASSESMENT**

### **PART A**

1. Which among the following is the most commonly used semiconductor?
  - a. Silicon
  - b. Carbon
  - c. Germanium
  - d. Sulphur
  
2. What happens to the resistance of a pure semiconductor when heated?
  - a. The resistance increases
  - b. The resistance decreases
  - c. The temperature remains the same
  - d. None of the above
  
3. How many valence electrons does a pentavalent impurity have?
  - a. 3
  - b. 4
  - c. 5
  - d. 6
  
4. How many valence electrons do trivalent impurities have?
  - a. 2
  - b. 3
  - c. 4
  - d. 5
  
5. Which of the following is created when trivalent impurities are added to a semiconductor?
  - a. Free electrons
  - b. Holes
  - c. Bound electrons
  - d. Valence electrons
  
6. A semiconductor in its purest form is called.....
  - a. Insulator
  - b. Superconductor
  - c. Intrinsic semiconductor

d. Extrinsic semiconductor

7. The temperature co-efficient of an intrinsic semiconductor is.....

- a. Zero
- b. Positive
- c. Negative
- d. None of them

### **PART -B**

1. Recall semi conductors with examples.
2. List out the properties of semi conductors.
3. Paraphrase the formation of holes and electrons through p-doping and n-doping.
4. Describe the mobility of electrons and Fermi level in semi conductors.
5. Describe the industrial applications of semi conductors.

### **PART -C**

1. Appraise the band theory of semi conductors with conduction and valance band.
2. Explain Types of semiconductors.
3. Classify semi conductors in optics and explain its features and applications?
4. Apply the knowledge of semiconductors in solar cells by elaborating the types of solar cells.
5. Explain Czochralski Process of single crystalline silicon synthesis

## **UNIT -II**

### **ELECTROCHEMICAL CELLS AND BATTERY TECHNOLOGY**

#### **2.1 INTRODUCTION**

In electrochemical cells, the chemical energy is converted into electrical energy. The cell potential is related to free energy change ( $\Delta G$ ). In an electrochemical cell, the system does work by transferring electrical energy through an electric circuit. Thus  $\Delta G$  for a reaction is a measure of the maximum useful work that can be obtained from a chemical reaction.

ie.,  $\Delta G = \text{maximum useful work}$

but we know that

Maximum useful work =  $nFE$

When a cell operates, work is done on the surroundings (flow of electricity).

$\Delta G = -nFE$  or  $\Delta G < 0$

Decrease in free energy is indicated by (-)ve sign.

One of the main uses of the galvanic cells is the generation of portable electrical energy. These cells are known as batteries.

**Galvanic cell (Daniel cell)**

An electrochemical cell that converts the chemical energy of spontaneous redox reactions into electrical energy is known as a galvanic cell or a voltaic cell.

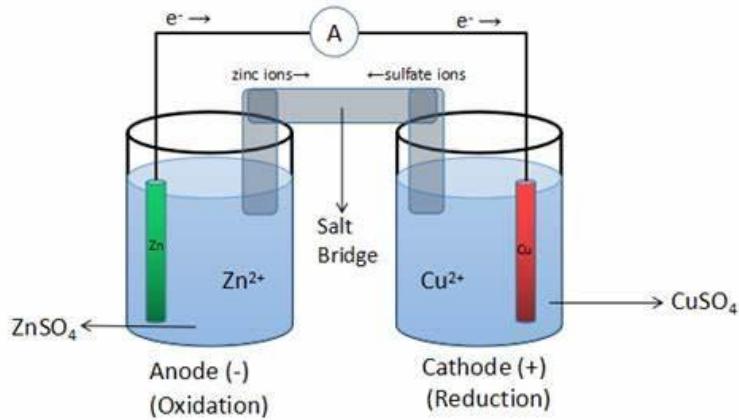
In oxidation-reduction reactions, electrons are moved from one species to another species. Energy is released if the reaction occurs spontaneously. Therefore, the released energy is used to do useful work. To tackle this energy, it is required to split the reaction into two separate half-reaction viz. oxidation and reduction. With the help of two different containers and wire, the reactions are put into them to drive the electrons from one end to the other end. This creates a voltaic cell.

#### **2.2 Galvanic cell (or) Daniel Cell**

##### **Principle**

Electric work done by a galvanic cell is mainly due to the Gibbs energy of spontaneous redox reaction in the voltaic cell. It generally consists of two half cells and a salt bridge. Each half cell further consists of a metallic electrode dipped into an electrolyte. These two half-cells are

connected to a voltmeter and a switch externally with the help of metallic wires. In some cases, when both the electrodes are dipped in the same electrolyte, a salt bridge is not required.



**Fig 2.1 Galvanic Cell (Voltaic Cell) Diagram**

#### Parts of Galvanic Cell

- **Anode** – Oxidation occurs at this electrode.
- **Cathode** – Reduction occurs at this electrode.
- **Salt bridge** – Contains electrolytes which are required to complete the circuit in a galvanic cell.
- **Half-cells** – reduction and oxidation reactions are separated into compartments.
- **External circuit** – Conducts the flow of electrons between electrodes
- **Load** – A part of the circuit utilizes the electron to flow to perform its function.

#### Working of Galvanic Cell

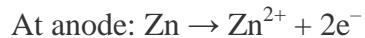
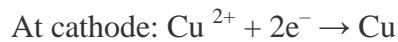
- In a galvanic cell, when an electrode is exposed to the electrolyte at the electrode-electrolyte interface, the atoms of the metal electrode have a tendency to generate ions in the electrolyte solution leaving behind the electrons at the electrode. Thus, making the metal electrode negatively charged.
- While at the same time metal ions in the electrolyte solution too, have a tendency to deposit on a metal electrode. Thus, making the electrode positively charged.

- Under equilibrium condition, charge separation is observed and depending on the tendencies of two opposing reactions, the electrode can be positively or negatively charged. Hence, a potential difference is developed between the electrode and electrolyte.
- This potential difference is known as electrode potential.
- Out of two electrodes, the electrode at which oxidation takes place is called anode while the electrode at which reduction takes place is called cathode.
- The anode has a negative potential with respect to the solution while the cathode has a positive potential with respect to the solution.
- Thus, a potential difference develops between two electrodes of the galvanic cell. This potential difference is known as cell potential.
- When no current is drawn from the galvanic cell, cell potential is known as the electromotive force of the galvanic cell.
- When the switch is set on, due to the potential difference, electrons flow from the negative electrode to the positive electrode.

### Example of Galvanic Cell

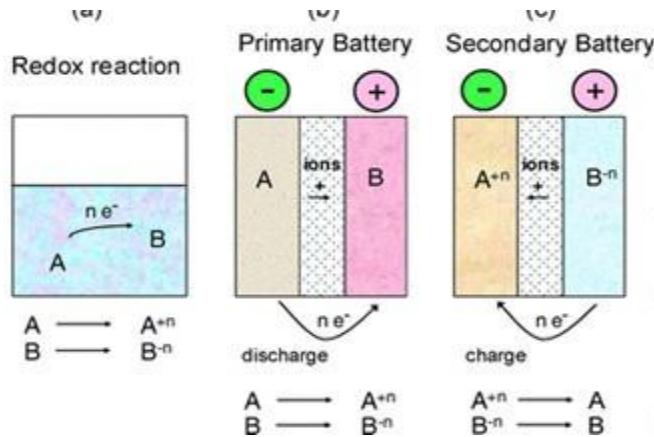
Electrochemical or galvanic cells were introduced as a tool for studying the thermodynamic properties of fused salts more than a century ago. Daniel's cell is an example of a galvanic cell that converts chemical energy into electrical energy. In Daniel's cell, copper ions are reduced at the cathode while zinc is oxidized at the anode.

Reactions of Daniel cell at cathode and anode are:



### 2.3 Batteries

*Battery* is electrochemical cells are connected in series that can be used as a source of direct electric current at constant voltages. A device which converts chemical energy to electrical energy is called battery connected together electrically in series. Batteries are commercial electrochemical cells.



**Fig 2.2 Diagram of battery**

### Advantages of batteries:

Batteries act as a portable source of electrochemical energy.

The portability of electronic equipment in the form of handsets has been made possible by batteries.

A variety of electronic gadgets have been made more useful and popular with the introduction of rechargeable storage batteries having reliability, better shelf life and tolerance to service.

For all commercial applications, batteries are constructed for their service. For example batteries for automotives and aircrafts, stand by batteries etc.

### Requirements of Battery:

- A useful battery should fulfill the following requirement
- It should be light and compact for easy transport.
- It should have long life both when it is being used and when it is not used.
- The voltage of the battery should not vary appreciably during its use.

#### 2.3.1 Classification of batteries

The galvanic or voltaic cells used as source of electrical energy are of three types:

- (i) Primary cells
- (ii) Secondary cells.
- (iii) Flow battery (or) Fuel cells

**(i) Primary battery (or) primary cells:** In these cells, the electrode and the electrode reaction cannot be reversed by passing an external electrical energy. The reactions occur only once and after use they become dead. Therefore, they are not chargeable.

Examples: Dry cell, Mercury cell.

### **ii) Secondary battery (or) Secondary cells**

In these cells, the electrode reactions can be reversed by passing an external electrical energy. Therefore, they can be recharged by passing electrical current and used again and again. These are also called storage cells (or) Accumulators.

Example

Lead acid storage cell, Nickel-cadmium cell.

### **iii) Flow battery (or) fuel cells**

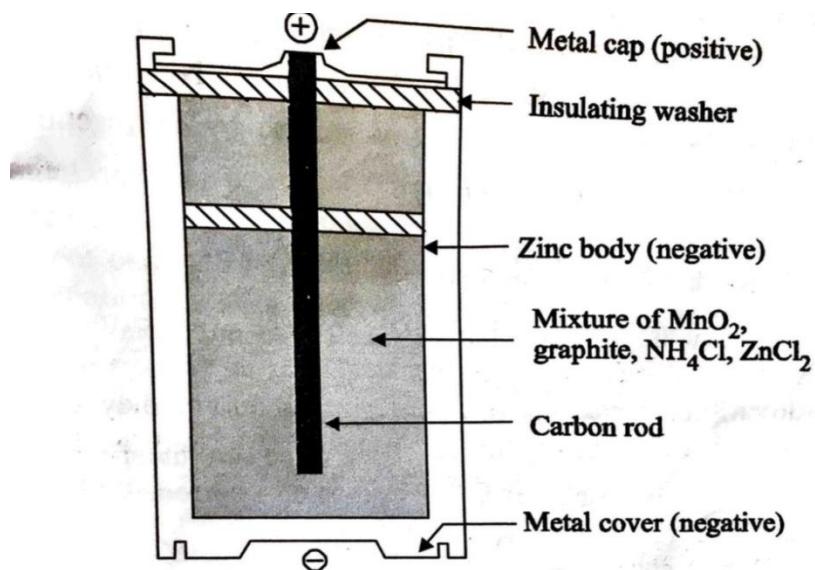
In these cells, the reactants, products and electrolytes are continuously passing through the cell. Here chemical energy gets converted into electrical energy.

Example

Hydrogen –oxygen fuel cell

#### **2.3.1.1 Dry cells (or) Leclanche's cell**

It is a primary cell, which works without fluid component.



**Fig 2.3 Dry cell (or) Laclanche cell**

Anode : Zinc can (or container or cylinder)

Cathode : Carbon (graphite) rod

Electrolyte :  $\text{NH}_4\text{Cl} + \text{ZnCl}_2 + \text{MnO}_2$

A dry cell consists of a zinc cylinder, which acts as anode. This zinc cylinder is filled with an electrolyte consisting of  $\text{NH}_4\text{Cl}$ ,  $\text{ZnCl}_2$  and  $\text{MnO}_2$  in form of paste using starch and water. A carbon rod (graphite), acts as cathode, is immersed in the electrolyte in the centre of the cell. The Zinc cylinder has an outer insulation of cardboard case. During use, the Zinc cylinder gets consumed and at the end, it will develop holes which are responsible for leakages.

## Working

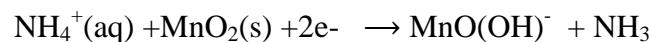
When the cell is working, Zinc loses electrons and a  $\text{Zn}^{2+}$  ion gets dissolved in the electrolyte. The electrons pass through the circuit and are consumed at cathode. This causes discharge of  $\text{NH}_4^+$  ions from the electrolyte.

### Cell reactions:

#### At anode:

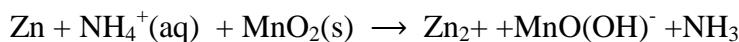


#### At cathode:



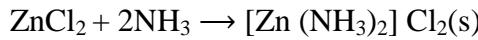
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#### Overall Reaction:



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In cathode reaction, Mn is reduced from +4 oxidation state to +3 oxidation state. The liberation of  $\text{NH}_3$  gas, which disrupts the current flow, is prevented by a reaction of  $\text{NH}_3(\text{g})$  with  $\text{Zn}^{2+}$  (from  $\text{ZnCl}_2$ ).



The voltage of Leclanche's cell is about 1.5V.

### Advantages

- The compact size of a dry cell makes it suitable for powering small electronic devices. ( toys,

flashlights, portable radios, cameras, hearing aids)

- The electrolyte used in dry cells is relatively not so harmful to the environment.
- Dry cells are inexpensive.

### **Disadvantages**

- This dry cell does not have an indefinite life, because  $\text{NH}_4\text{Cl}$  being acidic corrodes the zinc container, even if it is not used.
- When current is drawn rapidly from it, products build up on the electrodes, so voltage drop occurs.

### **Uses**

- It is used in transistor radios, calculators, Flash lights, torches etc.,

#### **1.3.1.2 Secondary cells:**

A secondary cell, once used can be recharged by passing current through it. It can be used over and over again. The redox reaction gets reversed during recharging. Since the electrical energy brings about the chemical change, it is converted into chemical energy. Thus electrical energy is stored in the form of chemical energy and utilized for supplying the current when needed. Secondary cells are also known as storage cells.

Whereas, a primary cell acts only as a galvanic or voltaic cell, a secondary cell can act both as galvanic cell and electrolytic cell. During discharging it acts as a galvanic cell, converting chemical energy into electrical energy and during charging it acts as an electrolytic cell converting electrical energy into chemical energy.

#### **a) Alkaline storage battery: Nickel-cadmium cell**

This is also a rechargeable battery.

#### **Description**

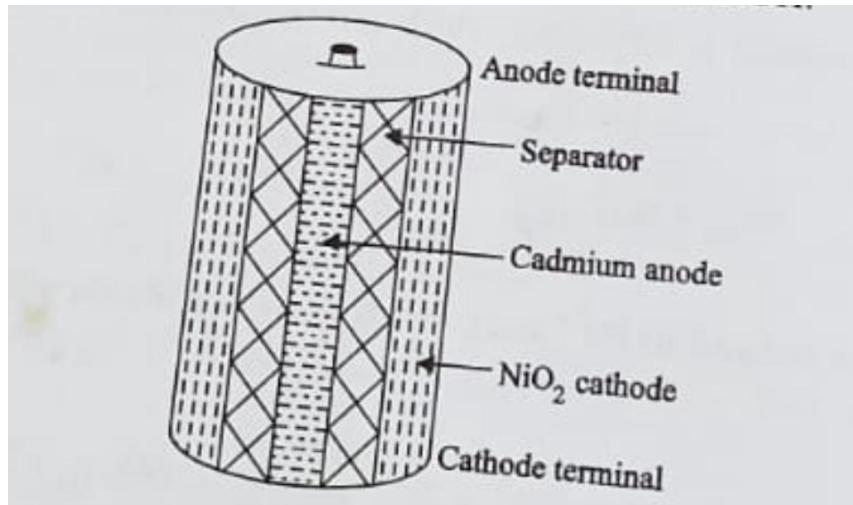
Nickel-cadmium cell consists of a cadmium anode and a metal grid containing a paste of  $\text{NiO}_2$  acting as a cathode. The electrolyte in this cell is KOH.

It is represented as:



### Working (Discharging)

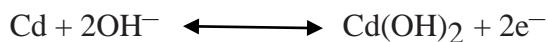
When the Nicad battery operates, at the anode cadmium is oxidized to  $\text{Cd}^{2+}$  ions and insoluble  $\text{Cd}(\text{OH})_2$  is formed. It produces about 1.4V.



**Fig 2.4 Nickel-Cadmium Battery**

At anode:

Cadmium is oxidized to  $\text{Cd}^{2+}$  and further it combines with  $\text{OH}^-$  ions to form  $\text{Cd}(\text{OH})_2$



At cathode:  $\text{NiO}_2$  is reduced to  $\text{Ni}^{2+}$  ions which further combine with  $\text{OH}^-$  ions to form  $\text{Ni}(\text{OH})_2$ .



Overall reaction during use (discharging):



From the above cell reactions it is clear that, there is no formation of gaseous products, the products  $\text{Cd}(\text{OH})_2$  and  $\text{Ni}(\text{OH})_2$  adhere well to the surfaces. This can be reconverted by recharging the cell.

### **Recharging the Battery**

The recharging process is similar to lead storage battery. When the current is passed in the opposite direction, the electrode reaction gets reversed. As a result, Cd gets deposited on anode and  $\text{NiO}_2$  on the cathode.

The net reaction during charging is



The open circuit potential of the cell ranges from 1.4 to 1.28V. It is compact, light weight battery with good cycle characteristics, capacity and long shelf life.

#### **Advantages:**

- It gives a constant voltage of 1.4V.
- It has a longer life than a lead acid battery.
- It is smaller and lighter.
- Like a dry cell, it can be packed in a sealed container.

#### **Disadvantages:**

- It is more expensive than lead storage battery.

#### **Uses:**

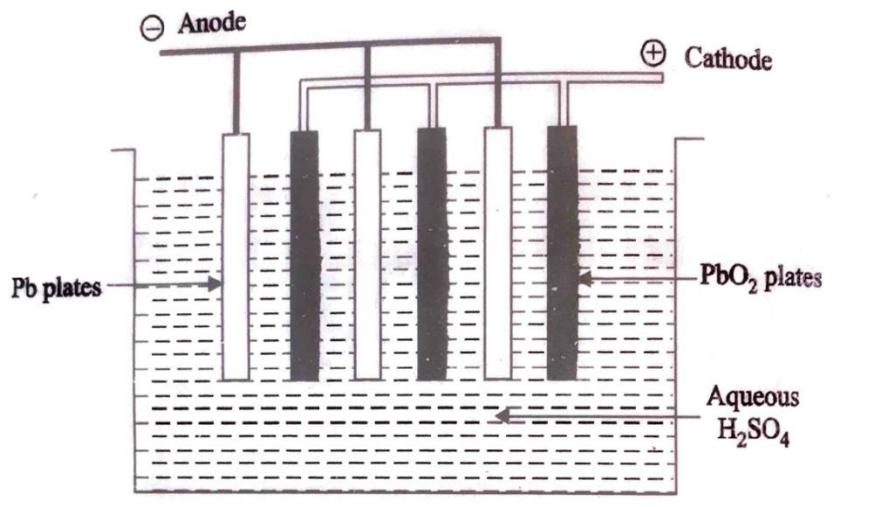
- It is commonly used in calculators, electronic, camera flashers, transistors, rechargeable flash lights and cordless appliances.

#### **Applications:**

Nickel cadmium cells are used in battery operated appliances such as pocket calculators, photo flash units, cordless garden tools, electric shavers, instruments, alarm systems, transmitters, receivers, emergency lighting, hearing aids, telemeters, etc.

### b) Acid storage battery (Lead acid battery)

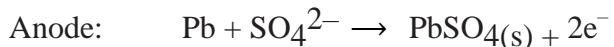
A simplified form of lead storage cell, the electrodes are lead grids. The anode grid is filled with spongy lead and the cathode grid is filled with lead dioxide ( $\text{PbO}_2$ ). A number of electrode pairs with inert porous partitions in between, are dipped in approximately 20% sulfuric acid, which is the electrolyte. The battery is encased in a plastic container.



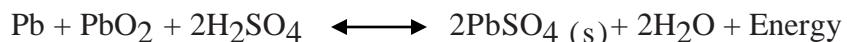
**Fig 2.5 Lead acid battery**

**Electrode reactions:** The electrode reactions that occur during the discharge of the cell, i.e., ondrawing current from the cell, are as follows:

The reactions are

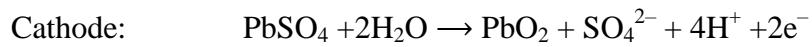


The overall reaction is



A single cell generates 2V and the six such cells in the battery produce a total of 12V.

**Recharge reactions:** The lead storage battery is rechargeable and is thus very useful. This is done by applying a voltage across the electrodes that is slightly higher than the voltage across the electrodes that is slightly higher than the voltage that the battery can deliver. The recharging involves applying an external negative voltage to the negative pole and a positive voltage to the positive pole of the cell. The sulphuric acid, consumed when the battery generates current is reformed. During recharging, the following reactions occur:



### **Advantages:**

- It is made easily.
- It produces very high current.
- The self-discharging rate is low when compared to other rechargeable batteries.
- It also acts effectively at low temperature.

### **Disadvantages:**

- The potential decreases with decrease in concentration of sulfuric acid.
- Excessive discharge and quick charging shortens the life of the battery.
- Cell potential and the effectiveness is reduced at low temperature.
- Excessive charging may damage the electrodes and may also lead to explosion

### **Uses:**

- Each electrode pair develops a potential of 2V. In order to obtain higher potential a number of electrode pairs are connected in series.
- Lead storage batteries are extensively used in automobiles to start the engine.
- It also used for electric supply in telephone exchangers, railway trains, hospitals, laboratories, etc., and for emergency power supplies.

### **2.3.1.3 FUEL CELL**

A fuel cell is an electrochemical which converts chemical energy contained in readily available fueloxidant system into electrical energy.



**Examples:** 1.  $\text{H}_2\text{-O}_2$  fuel cell

2.  $\text{CH}_3\text{OH}\text{-O}_2$  fuel cell

## Hydrogen-Oxygen fuel cells:

Hydrogen –Oxygen fuel cell is the simplest and most successful fuel cell, in which the fuel-Hydrogen and the oxidizer – oxygen and the liquid electrolyte are continuously passed through the cell.

### Description

It consists of two porous electrodes anode and cathode. These porous electrodes are made of compressed carbon containing a small amount of catalyst (Pt, Pd, and Ag). In between the two electrodes an electrolytic solution such as 25% KOH or NaOH is filled. The two electrodes are connected through the volt meter.

### Working

Hydrogen (the fuel) is bubbled through the anode compartment, where it is oxidized. The oxygen (oxidizer) is bubbled through the cathode compartment, where it is reduced.

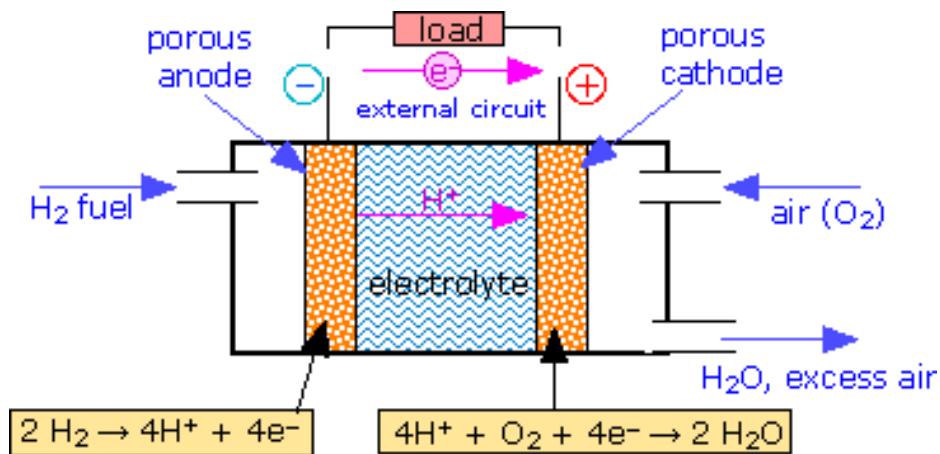
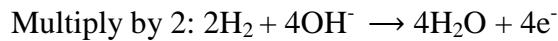
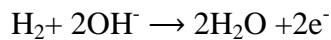


Fig 2.6 Hydrogen – Oxygen Battery

### Various reactions

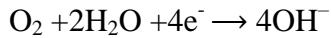
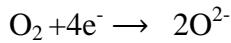
#### At anode

Hydrogen gas, passed through the anode, is oxidized with the liberation of electrons which then combine with hydroxide ions to form water.

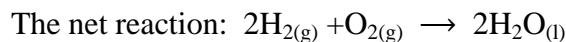
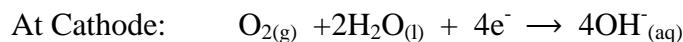
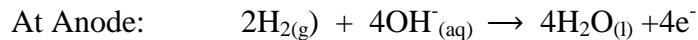


### At cathode

The electrons, produced at the anode, pass through the external wire to the cathode where it is absorbed by oxygen and water to produce hydroxide ions,



### Overall cell reaction



The standard emf of the cell,

$$E^0 = E^0_{\text{ox}} + E^0_{\text{red}} = 0.83\text{V} + 0.40\text{V} = 1.23\text{V}$$

## **Advantages**

- The energy conversion is very high (75-82%).
- Fuel cell minimizes expensive transmission lines and transmission losses.
- It has high reliability in electricity generation.
- The byproducts are environmentally acceptable.

## **Disadvantages**

- Expensive to manufacture due the high cost of catalysts( Platinum)
- Lack of infrastructure to support the distribution of hydrogen
- A lot of the currently available fuel cell technology is the prototype stage and not yet validated
- Hydrogen is expensive to produce and not widely available.

## **Uses**

- The electrolyte used in these cells is lithium potassium carbonate salt. This salt becomes liquid at high temperatures, enabling the movement of carbonate ions.
- The anode and the cathode of this cell are vulnerable to corrosion due to the high operating temperature and the presence of the carbonate electrolyte.
- These cells can be powered by carbon-based fuels such as natural gas and biogas.

## **Application**

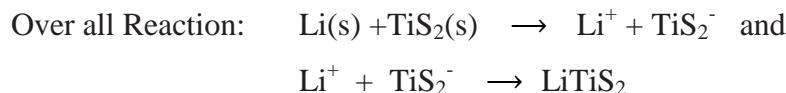
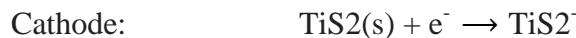
- Hydrogen –Oxygen fuel cell are used as auxiliary energy source in space vehicles, submarines or other military- vehicles.
- The weight of the fuel battery sufficient for 15days in space is approximately 250kg.
- In case H<sub>2</sub>-O<sub>2</sub> fuel cells, the product water proved to be a valuable source of fresh water by the astronauts.

## 2.4 SOLID STATE BATTERY

A solid-state battery is a battery technology that uses solid electrodes and a solid electrolyte, instead of the liquid or polymer gel electrolytes found in lithium-ion or lithium polymer batteries. Materials proposed for use as solid electrolytes in solid-state batteries include ceramics (e.g., oxides, sulfides, phosphates), and solid polymers.

### 2.4.1 LITHIUM BATTERY

It is regarded as the battery of the future. It is a solid state battery. It uses a solid electrolyte and not a solution or paste. Anode is lithium. Cathode is  $\text{TiS}_2$ . The solid electrolyte used in this is a polymer which permits the passage of ions but not that of electrons. The cell reactions are



The cell is rechargeable and produces a cell voltage of 3v

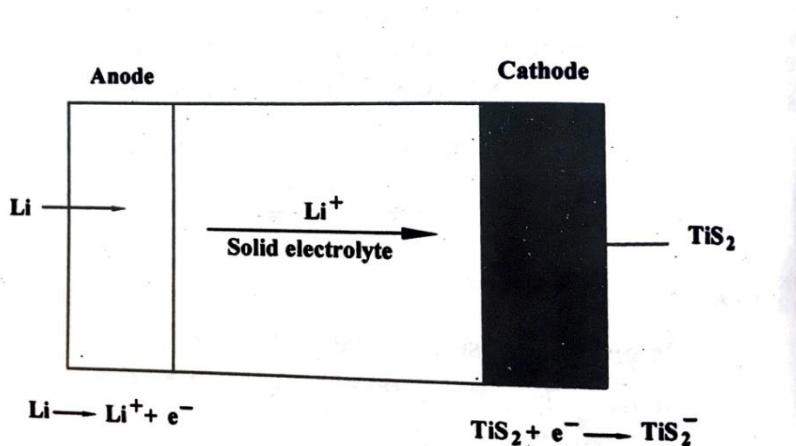


Fig 2.7 Lithium battery

### Advantages

The lithium is considered to be the cell of the future because,

- Its cell voltage is high, 3.0V.
- Lithium being a light metal, only 7g (1 mole) material is just sufficient to produce 1 mole of electron.
- Li has the most negative  $E^\circ$  value and, hence, generates a higher voltage than other types of cells.

- All the constituents of the battery are solids and hence there is no risk of leakage from the battery.
- This battery can be made in a variety of sizes and shapes.

### **Disadvantages**

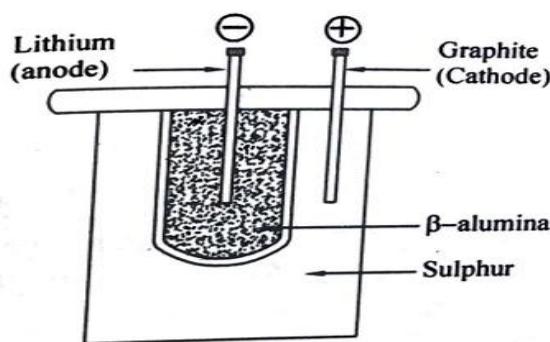
- For lithium – ion batteries, it needs the protection circuit to maintain voltage.
- The transportation of large amounts of lithium batteries comes under regulatory provisions that lead to transportation restrictions.
- The manufacturing of lithium batteries is costlier than nickel-cadmium.
- Lithium-ion batteries suffer the issue of ageing.
- The lithium- ion batteries are considered to be an immature technology.

### **Uses**

- Lithium –ion are rechargeable and used in vaping devices, many personal electronics such as cell phones, tablets, laptops, E-bikes, electric tools etc.,

### **2.4.2 LITHIUM SULPHUR BATTERY**

Another lithium battery is lithium sulphur battery. Here, the anode is Lithium. Sulphur is the electron acceptor. The electron from Li is conducted to S by a graphite anode.  $\beta$ -alumina is used as the solid electrolyte.



**Fig 2.8 Lithium Sulphur battery**

This battery is operated at high temperatures as Li and S must be in the molten states for the operation of the following cell reactions.



The  $\text{S}^{2-}$  formed reacts with elemental sulphur to form polysulphide ion. The direct reaction between Li and S, detrimental to current production, is prevented by the intervening alumina in the cell.

### **Advantages**

- It has light weight.
- It has a high energy density.
- It is used in electric cars.

### **Disadvantages**

- Transportation of Lithium Sulphur batteries is one of the major limitation. Because of the chemicals used in them, nearly every airline company restricts lithium sulphur batteries to carry in the aircraft.
- Lithium Sulphur batteries, relative to other batteries, are quite costly. This is another limitation of these batteries.
- You will buy nearly 2 to 3 lithium ion batteries as much as you get a Lithium Sulphur battery at the same cost.

### **Uses**

- Lithium- sulphur cells are already used in devices that demand light weights batteries
- It can run for a long time off a single charge, such as drones or satellites.

## **SELF ASSESMENT**

### **PART A**

1. Select the anode used in dry cell.
  - a) Zinc
  - b) Graphite
  - c) Mercury(II)oxide
  - d) Nickel
2. Which of the following cell has a reversible chemical reaction?
  - a) Lead-acid
  - b) Mercury oxide
  - c) Carbon-zinc
  - d) Silver-oxide
3. Write the final oxidation state of manganese after the electrochemical reactions in a dry cell?
  - a)+4
  - b)+3
  - c)+2
  - d)+1
4. Recognize the electrolytic solution used in a hydrogen-oxygen fuel cell.
  - a) 75% KOH solution
  - b) 25% KOH solution
  - c) 75% NaOH solution
  - d) 25% NaOH solution
5. Label the conversation of chemical energy in fuel cell.
  - a) Solar
  - b) Electrical
  - c) Potential
  - d) mechanical

6. What is the standard emf of the hydrogen-oxygen fuel cells?

- a) 3.96 V
- b) 1.23 V
- c) 0.58 V
- d) 2.54 V

7. Which is the material used as anode in a lithium battery?

- a) Brass foil coated with graphite
- b) Aluminum foil coated with graphite
- c) Copper foil coated with graphite
- d) Stainless steel coated with graphite

### **PART -B**

1. Write the classification of energy storage devices with examples.
2. Explain the construction and workings of Leclanche's cell.
3. With a neat sketch explain the function of Hydrogen-Oxygen fuel cell.
4. Illustrate the construction and working of Lithium battery.
5. Write notes on Lithium Sulphur battery.

### **PART -C**

1. Describe construction and working of Galvanic Cell with neat diagram.
2. Discuss the construction and working of lead acid storage battery with reaction occurring during charging and discharging.

3. Illustrate the working of Nickel- Cadmium battery and explain its functioning during discharging and recharging.
4. Paraphrase the fuel cell, with the functioning of Hydrogen –Oxygen fuel cell.
5. Explain Lithium and Lithium sulphur batteries with neat diagram.

## **UNIT III- DEVICE CORROSION**

### **3.1 Introduction**

Corrosion is the destructive attack of a metal by chemical or electrochemical reaction with its environment, chemical attack accompanies physical deterioration. Corrosion causes the malfunctioning of controls and switching gear that results in more than 50% of electrical system downtime, causing a huge loss. Harsh environments can cause electrochemical deterioration and chemical attack on metallic wire terminals. Overall, the corrosion of current-carrying parts and switching, as well as controlling equipment, affects the reliability and uninterrupted operation of all kinds of electrical components and production facilities. This type of corrosion caused to electrical and electronic devices are called as Device Corrosion.

The careful selection of coatings and substrate materials based on the service exposure of electrical equipment and controls can improve the reliability and cost effectiveness of the entire system. Electronic devices are presently used under service conditions that were never thought off few years back. Consumer electronics are used under highly variable environmental parameters (e.g. mobile phones brought to the seaside or sound system installations in kitchens or bathrooms).

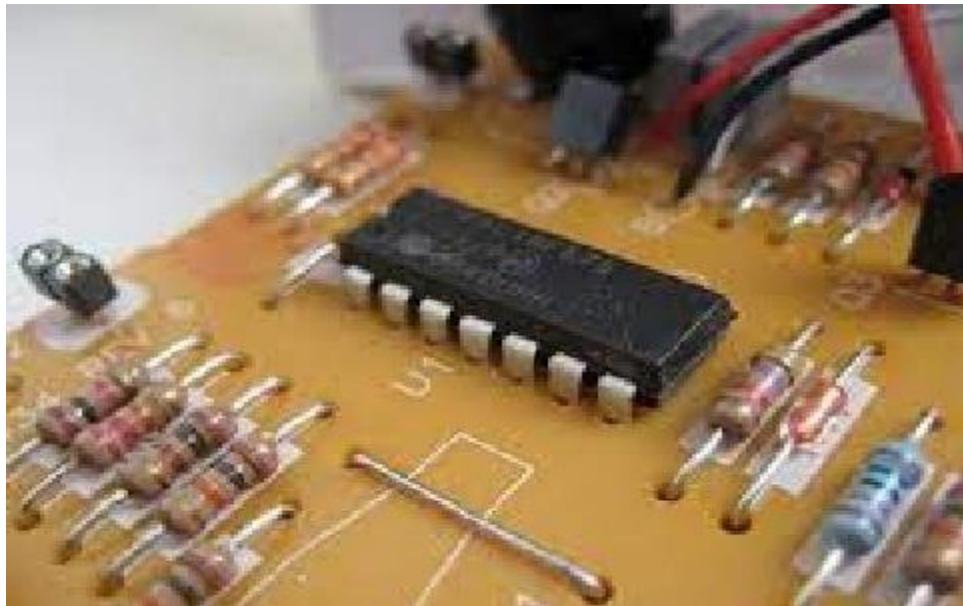
Industrial electronics also experience a variety of environments due to their wide spread use. In many cases precautions for protecting electronics against aggressive conditions are not met. The demand for electronics is not lifetime performance, but reliability, since replacing electronics is a costly task. The increased use of electronics has also increased the demand for corrosion reliability. Corrosion failures can be difficult to diagnose and cause unexpected production loss due to plant shut down. Overall size of electronic equipment and therefore the component size have been decreasing at a faster rate.

### **3.2 Chemistry of IC (Integrated Circuit)**

The chemistry involved in fabrication of IC (fig 3.1) chips:

- Substrate preparation
- Epitaxial growth
- Silicon dioxide growth
- Photo-etching

- Diffusion



**Fig.3.1 Integrated circuit and related components**

### 3.2.1 Substrate Preparation

It involves the following steps:

**Selection of Raw Material:** Silicon of about 98% purity is obtained on reduction of silicon dioxide on heating it along with carbon at a suitably high temperature in a furnace.

**Zone refining:** The order of purity needed in manufacture of IC chips is 1 impurity atom in  $10^9$  silicon atoms. This high order of purity is obtained on repeated zone refining process.

**Crystal Growth:** Silicon of desire purity is heated in a furnace and p-type impurity in proper proportion is added to it. The p-type silicon crystal is then grown from the melt using a seed crystal.

**Slicing and Polishing:** The p-type silicon crystal is sliced into wafer each of thickness about 6 mils. Each wafer is then lapped to remove saw marks and then polished mechanically or chemically to produce mirror like smoothness.

### 3.2.2 Epitaxial Growth

- Epitaxial growth consists in formation of a single crystal thin film from the gas phase on a wafer (p-type in this case) of the same material (silicon). This epitaxial layer forms a continuation of the single crystal structure of the substrate.
- Epitaxial growth uses a chemical reaction whereby silicon is precipitated from a gaseous solution to form a thin film of single crystal (mono crystalline) silicon on the surface of silicon wafer placed in the gaseous solution.
- The basic chemical reaction involved in epitaxial growth of pure silicon is hydrogen reduction of silicon tetrachloride .The epitaxial layer may be made either n-type or p-type.

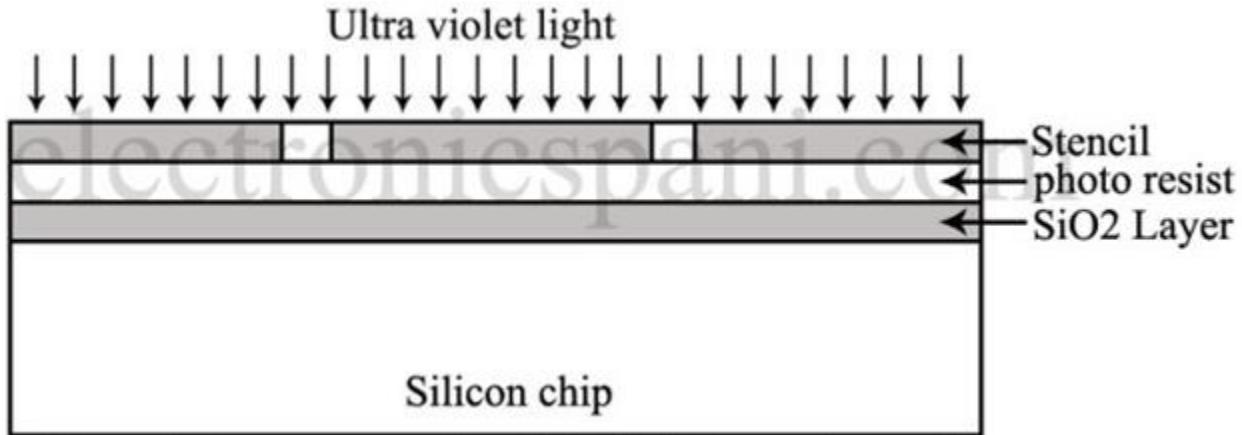
### **Salient Features of Epitaxial Process**

- The atom is arranged on crystal substrate in the single crystal fashion forming an extension of the substrate layer.
- Epitaxial layer is grown from gas phase whereas large size crystals are grown from liquid phase. Further, in epitaxial process, no part pf the system has temperature approaching the melting point.
- Epitaxial layer has highly uniform resistivity (better than disused layer).
- Epitaxial layer may also be grown on diffused surface.
- Doping may be either p-type or n-type.
- Doping concentration may be varied over large range and complex impurity profile may be grown.

### **3.2.3 Silicon Dioxide Growth**

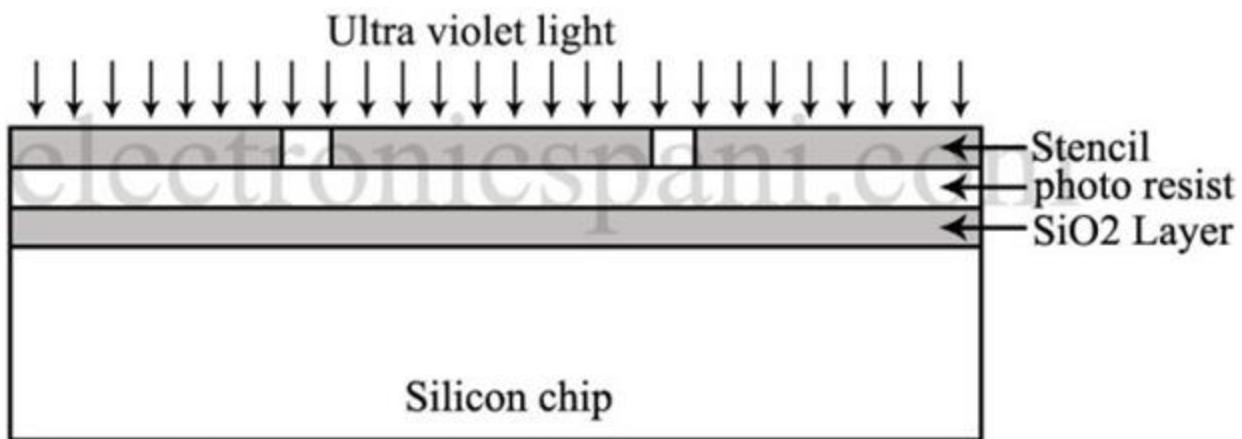
Before formation of a fresh  $\text{SiO}_2$  layer on the wafer surface, the wafer is washed in a suitable solution to remove the previous  $\text{SiO}_2$  layer. Then the wafer is heated to a suitably high temperature in an atmosphere of oxygen. Silicon oxidises to form a thin layer of  $\text{SiO}_2$ .

### **3.2.4 Photo-Etching**



**Fig.3.2 Photo-Etching Process**

- The wafer (also called a slice or substrate) with top of SiO<sub>2</sub> layer is first coated with a uniform layer of some photo-sensitive emulsion such as kPR (kodak photo-resist).
- An enlarged black and white pattern of desired opening in first made and then reduced photographically to proper small size to form a mask or stencil (or negative). This stencil or mask is then placed over the photo-resist Ultra-violet light is then made incident on the mask. The photo-resist under the transparent region of the stencil gets polymerized as shown in figure 3.2



**Fig.3.2 Photo-Etching Process**

- The stencil is then removed and then wafer is developed using suitable chemical such as trichloroethylene to dissolve the unexposed or un polymerized portion of the photo-resist film leaving unaffected the desired pattern of polymerized photo resist as shown in figure 3.3.



**Fig.3.3 Polymerised photo resist**

- The unremoved portions of photo-resist are then fixed or cured making them resistant to corrosive etching process.
- The chip is now immersed in an etching solution of hydrofluoric acid. The acid dissolved the SiO<sub>2</sub> from the portions unprotected by the photo-resist pattern.
- Next, the impurities are diffused through these unprotected portions.
- After photo-etching and diffusion, the resist mask and the underneath SiO<sub>2</sub> layer are removed using chemical solvent such as sulphuric acid and in addition by mechanical abrasion.

### 3.2.5 Diffusion of Impurities

- This forms the most important process in the manufacture of IC chips.
- Steps involved in Diffusion Process
- Dopant atoms in high concentration are brought in contact with the surface of the silicon wafer for a suitably short period of time.
- Next the dopant is removed leaving behind some dopant atoms on the wafer surface.
- The wafer is now heated at a suitably high temperature. Due to heating the dopant enters the wafer surface i.e. dissolves in the solid-state silicon crystal.

The depth to which the dopant on (i) original concentration of dopant (ii) nature of dopant (iii) temperature and (iv) duration of heating.

### **Salient Features of Diffusion Process**

- Dopant atoms enter the crystal without damaging the crystal structure. In alloying, on the other hand, crystal structure gets damaged.
- Diffusion process has to be performed several times since a number of circuit elements are normally needed to be fabricated simultaneously.

During the second diffusion at a higher temperature, the diffusion of the first dopant may take place again. Hence, it is necessary to fix proper sequence of different dopants.

A few dopants have diffusion constants much greater in silicon than in SiO<sub>2</sub>. In such a case, SiO<sub>2</sub> layer may be used as a mask in diffusion process. However, the SiO<sub>2</sub> layer itself is produced by diffusion process. However, the SiO<sub>2</sub> layer itself is produced by diffusion at a higher temperature of 900°C to 1300°

Diffusion may take place both perpendicularly and sideways or slanting. The slanting diffusion permits dopant to enter region below the SiO<sub>2</sub> layer. This part of the resulting pn junction is then free from exposure to the contaminating atmosphere.

### **3.3. Chemistry of PCB (Printed Circuit Board)**

#### **3.3.1 Parts of Printed Circuit Board**

There are four parts to a printed circuit board:

**Substrate:** The substrate is made of fibreglass, the “skeleton of the PCB.” Fiberglas provides core strength to the printed circuit board and helps resist breakage.

**Copper Layer:** Depending on the board type, this layer can either be copper foil or a full-on copper coating. The copper layer’s function is to carry electrical signals to and from the PCB like your nervous system carries signals between your brain and muscles.

**Solder Mask:** The solder mask is a layer of polymer that helps protect the bare copper so that it doesn’t short-circuit from coming into contact with the environment. The solder mask acts as the PCB’s “skin.”

**Silkscreen:** The silkscreen is usually on the component side of the PCB board and is used to show part numbers, logos, symbols switch settings, component references, and test points. The silkscreen can also be known as legend or nomenclature.

### 3.3.2 PCB Manufacture process

PCB manufacturing involves several chemical processing steps such as electrochemical or electro less plating and etching/stripping of metal-layers or application of photo resist. Also drilling of vias and through-holes are steps in a manufacturing process:

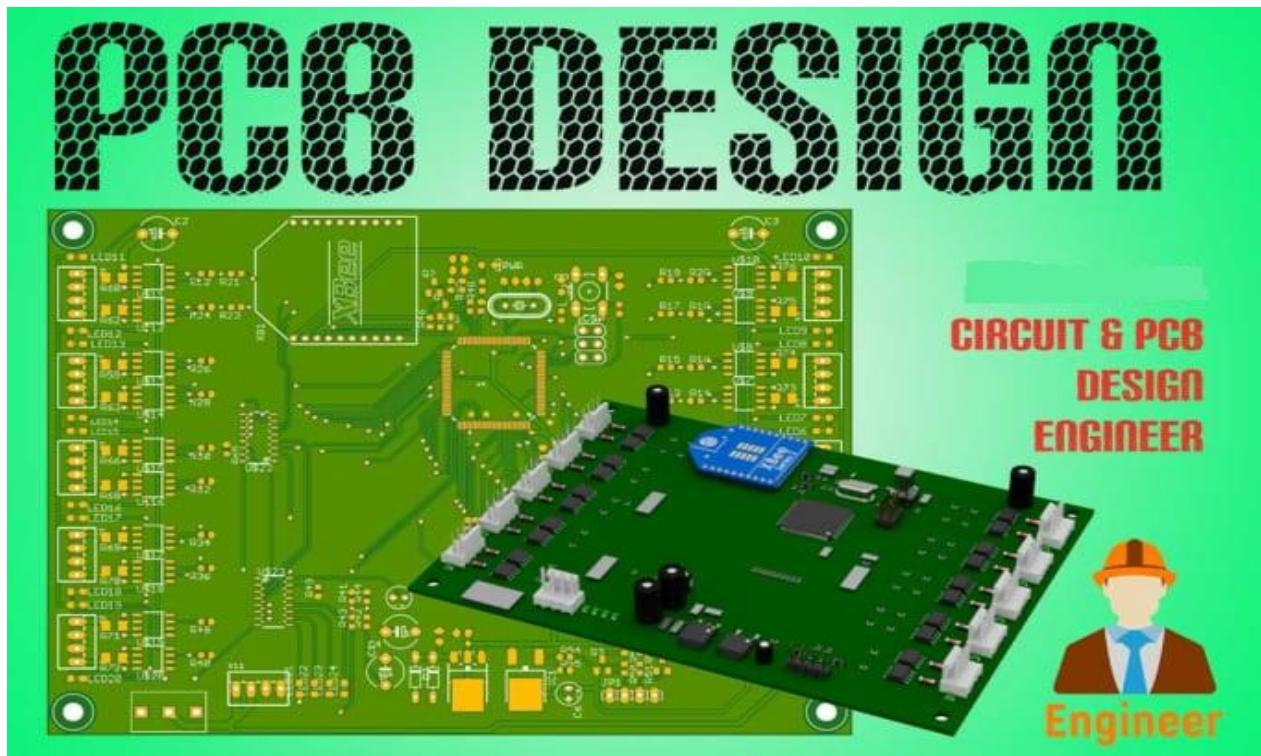


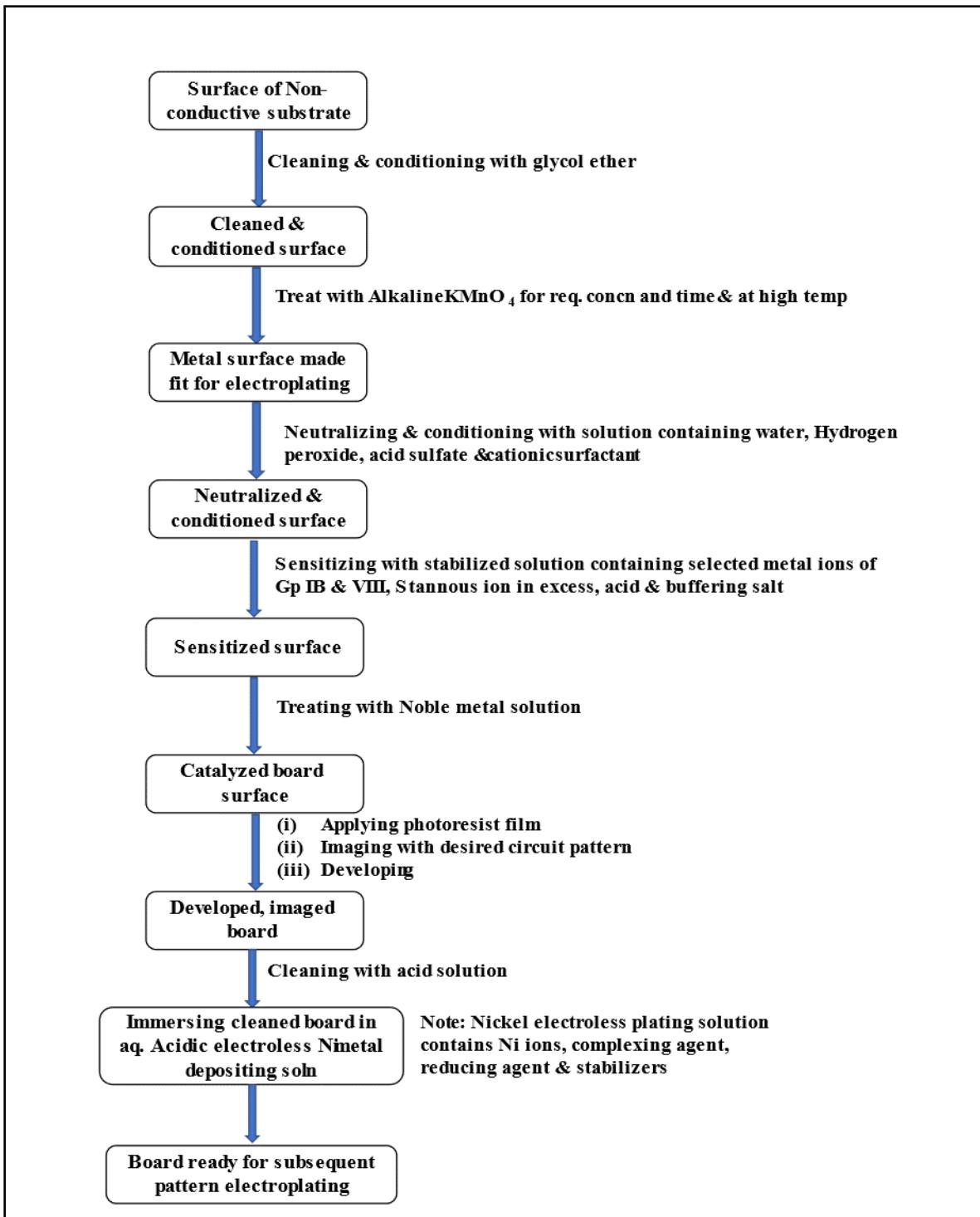
Fig: 3. 4 Design of PCB (Printed Circuit Board)

#### 3.3.2.1 Electro less plating

An electroless plating process comprising the following steps

- Contacting a surface of a non-conductive substrate with a cleaning and conditioning composition comprising at least one glycol ether;

- b) Treating the cleaned and conditioned surface resulting from step a) with an alkaline permanganate solution for a time, at a concentration, and at an elevated temperature sufficient to prepare such surface for a metal lay to be subsequently applied by electroplating;
- c) Contacting the surface resulting from step b) with an aqueous neutralizing and conditioning solution comprising water, hydrogen peroxide, at least one acid sulfate compound and at least one cationic surfactant;
- d) Contacting the surface resulting from step c) with a stabilized sensitizing solution comprising (i) ions of a metal selected from the group consisting of Group VIII and IB transition metals, (ii) stannous ions present in the solution in a molar concentration in excess of the concentration of said metal ions, (iii) an acid and (iv) a buffering salt;
- e) Contacting the sensitized surface resulting from step d) with a solution containing a noble metal salt to thereby catalyze the surface for subsequent electroless metal plating;
- f) Contacting the board resulting from step e) with a dry film photoresist, imaging the resulting board with a pattern corresponding to a desired circuit pattern and developing the imaged board;
- g) Contacting the developed, imaged board resulting from step f) with an acidic cleaning solution; and
- h) Immersing the board resulting from step g) in an aqueous acidic electroless nickel metal depositing solution, for a time, at a concentration and at a temperature sufficient to prepare the board for subsequent pattern electroplating, said aqueous acidic electroless nickel metal depositing solution comprising (i) nickel ions, (ii) a complexing agent (iii) a reducing agent capable of reducing the nickel ions to nickel metal in an acidic state, provided said reducing agent does not contain any formaldehyde or formaldehyde-generating composition and (iv) one or more stabilizers.



Flow chart of electroless plating in PCB fabrication

### **3.3.2.2 Etching/Stripping of Metal-Layers**

#### **Step 1: Sketch a Schematic and Check the Math**

Sketch out a circuit and track down all required components.

#### **Step 2: Input your Design into a PCB Design Software**

Programs such as Eagle and Easy EDA allow to design the schematic PCB

#### **Step 3: Transfer the Layout to the Board**

To ensure an accurate transfer, tape this print out over top of a copper clad laminate PCB. Using a pushpin, stab through the paper where each component lead will penetrate the board. This will leave dots on the copper where these components go. The small indentation on the copper will also help the drill bit find the exact location the lead will go. Remove the printed sheet and make sure all components are marked on the copper. Use a 1/32" (maximum) bit to drill out the holes that were marked on the board. Once all the holes are drilled, clean the top of the copper plate with a piece of sandpaper. Using a permanent marker, draw traces between all the components referencing the printed PCB layout. Allow some time for the ink to dry and touch up the board where the marker is faint.

#### **Step 4: The Etching Process**

Once the second coat of marker is completely dry it is time to give the board a bath in ferric chloride. Ferric chloride is a corrosive, acidic chemical compound that will eat away all copper on the board that is not protected by the marker's ink. Pour a modest amount of ferric chloride into a plastic container with a lid; just enough to cover the board completely. Let the board soak for 10 minutes, make sure the lid is properly secured and agitate it every few minutes by rocking the container back and forth. After 10 minutes inspect the board and if no copper is visible, remove the board while wearing a latex glove. Pat the board dry with a disposable rag to remove all ferric chloride from the board. Rinse the board with acetone that will make quick work of the marker ink to reveal your unharmed traces. The etching process is complete!

#### **Step 5: Populate the Board and Test Your Circuit**

After the board has been etched, use a multimeter to do a continuity test.

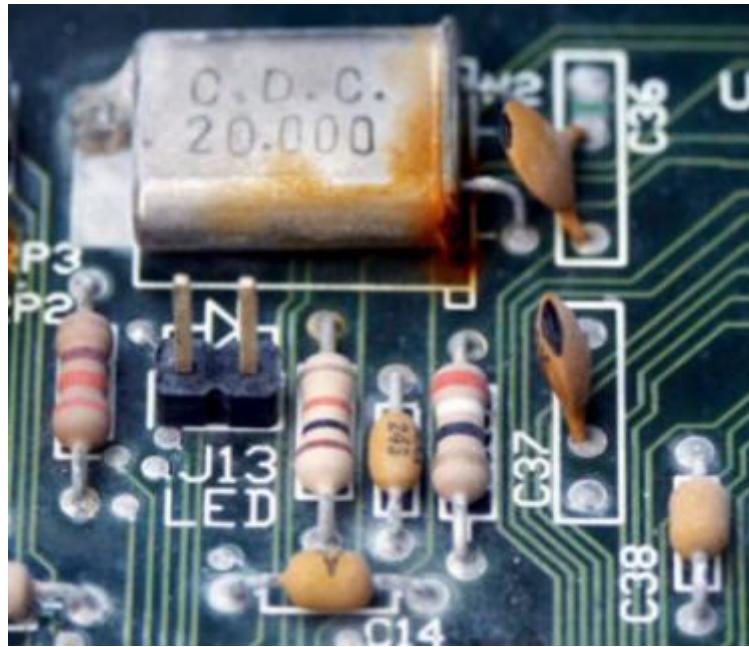
### **3.3.2.3 Drilling of vias**

PCB drilling (which is also known as printed circuit board drilling), is the process of creating holes, slots and other cavities in an electronic circuit board. During the PCB drilling process, a number of different hole types are drilled. Vias terms about that they provide the connections between different layers of a circuit board. Used to electrically and thermally join traces, pads, and polygons on different layers of a PCB. Vias are copper cylinders that are placed or formed in holes that have been drilled in a PCB.

## **3.4 Causes of Corrosion on IC,PCB**

### **3.4.1 General causes of corrosion in electronic devices**

1. The materials and miniaturization has significantly contributed to the corrosion of electronic system.
2. The exposure of electronics to environments where temperature, humidity and atmospheric pollutants such as chlorides,  $\text{NO}_x$ ,  $\text{SO}_x$ , and hydrogen sulphide ( $\text{H}_2\text{S}$ ), which are not controlled, can result in atmospheric corrosion of the metallic components .
3. Among the environmental issues, a significant problem is the residues found on the PCBs. These residues are the contamination on the surface due to the remains of the chemicals used for the manufacturing process. This could be the left over of original chemicals or decomposed fractions of a compound formed during the production cycle. These are the fluxing agents,
4. Flux residues are one of the most common and harmful residue sources that affect the reliability of PCB assemblies, and field failures regularly occur due to flux residues that have not been activated properly or not removed during assembly.
5. The most common flux residues are the activating species such as chloride and weak organic acids, but also additives and surfactants like polyglycols are found to reside and create problems in electronic assemblies ( figure3.5)



**Fig :3.5 Corrosion of electronic systems**

### **3.4.2. Miniaturization**

Miniaturization is the trend to manufacture ever smaller mechanical, optical and electronic products and devices. In electronics, the exponential scaling and miniaturization of silicon MOSFET (metal–oxide–semiconductor field-effect transistor, or metal–oxide–silicon (MOS )transistors leads to the number of transistors on an integrated circuit chip doubling every two years. This leads to MOS integrated circuits such as microprocessors and memory chips being built with increasing transistor density, faster performance, and lower power consumption, enabling the miniaturization of electronic devices.(Fig.3.6)

Examples include miniaturization of mobile phones, computers and vehicle engine downsizing.

The miniaturization of electronic systems and the increase in their usage has augmented the risk of corrosion in electronics devices. The demand for miniaturized devices has resulted in higher density packing with reduction in component size, closer spacing, and thinner metallic parts.

Material loss of the order of nano-grams can cause reliability problems.

Miniaturization and the requirement for high component density has resulted in smaller components, closer spacing, and thinner metallic paths. Thus, the effect of bias potentials and small defects is magnified.



**Fig .3.6 Miniaturization of Medical device**

### **3.4.3 Complex material Utilization**

#### **Micro pitting on Aluminium on IC During Processing**

Aluminium metallization, alloyed with copper, can form intermetallic A12Cu compounds along the grain boundaries, which act as cathodic sites relative to the aluminium adjacent to the grain boundaries. This leads to dissolution of an aluminium matrix in the form of micro pitting during the rinsing step after chemical etching.

#### **Corrosion of Aluminium by Chlorinated/Halogenated Solvents**

Both liquid and vapor-phase halogenated solvents used for production of ICs and PCs readily corrode aluminum-containing components. Water contamination of the solvents increases the time-to-corrosion on the one hand; however, on the other hand, it increases the subsequent corrosion rate. Dilution of the stabilized solvents with aromatic or alcohol solvents leads to the breakdown of the halogenated solvent and the formation of chloride ions, which corrode aluminium and aluminium-copper alloys.

#### **Solder Corrosion**

The corrosion resistance of lead-tin solder in aqueous and gaseous environments is a function of the alloy composition. It improves significantly when the tin content increases. Lead forms unstable oxides, which easily react with chlorides, borates, and sulfates.

### **3.4.4 Production and Service factors**

#### **3.4.4.1 Production Related Contamination**

Production related contamination can be present on any electronic device due to chemical compounds contained in the bare printed circuit board (PCB) substrate or compounds resulting from various processes during PCB manufacturing process (figure.3.7).

##### **Polymer additives in PCB substrate**

Polymer additives used in PCB substrate production can also cause surface contamination of the substrate, which can affect the performance of components that are directly attached to the surface.

##### **Etching and plating**

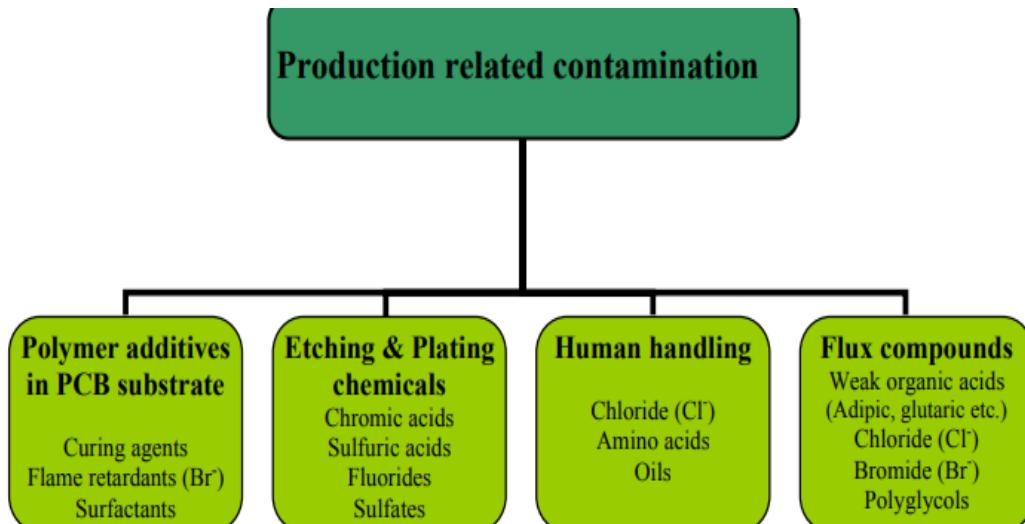
The metal plating process that involves Chromic acid, sulphuric acid , fluorides and sulphates also cause corrosion.

##### **Human handling**

Human handling of PCBs can also occur during production, and this is likewise a potential source of contamination resulting from fingerprints, skin oils, saliva, dandruff etc. Especially fingerprints (containing chlorides, amino acids etc.) can be an accelerator of electronic corrosion

##### **Flux Compounds**

The most common flux residues are the activating species such as chloride and weak organic acids, but also additives and surfactant's like poly glycols are found to reside and create problems in electronic assemblies.



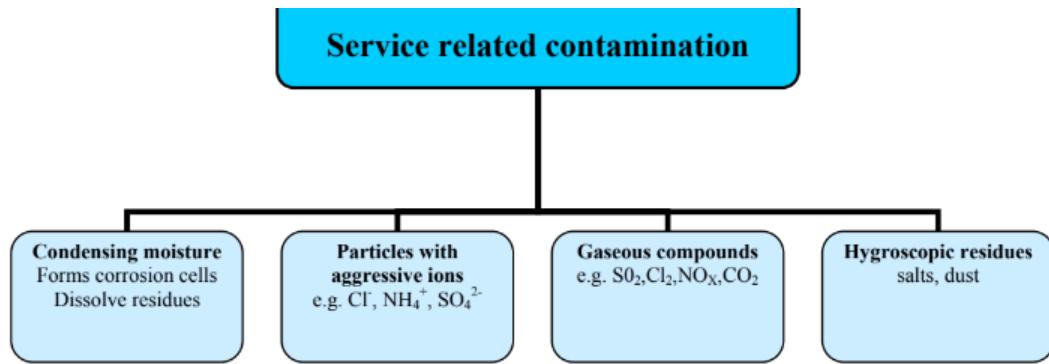
**Fig: 3.7 Production Related Contamination**

#### 3.4.4.2 Service Related Contamination

Humidity contributes to corrosion by the process of Ion migration. When voltage is applied to the metal in electronic equipments, the water molecules from the air (humidity) that have settled onto the metal surface causes the metal ions to elute.

The exposition of these devices to environments where temperature, humidity and atmospheric pollutants like chlorides,  $\text{NO}_x$ ,  $\text{SO}_x$ , COS and hydrogen sulfide ( $\text{H}_2\text{S}$ ) which are not completely controlled, can favor atmospheric corrosion on their metallic components. Small quantities of corrosion products are enough to induce reliability issues and even catastrophic failures in the microelectronic devices due to the formation of insulating layers by the corrosion film.

Dust may cause electrical leakage, shorting and opening of PCBs under different conditions. A conductive electrolyte film can be formed, which can degrade the surface insulation resistance between conductors. Dust particles can increase friction on contacting surfaces, thus promoting third body wear and fretting corrosion, which in turn can change the contact resistance. Dust particles act as dielectric materials to induce signal interference in the contaminated signal connectors and lines. Dust accumulation on the heat sink, power connectors, or active devices can cause overheating ( fig 3.8)



**Fig:3.8 Service Related Contamination**

### 3.4.5 Environmental Contamination (Air borne contamination)

One of the most common reasons for electronic failure is environmental contaminants and conditions.

The list of contaminants includes fine and coarse particles of such species as chlorides, sulfates, sodium, ammonium, potassium, magnesium, and calcium. The single most important environmental condition affecting the impact of particulate matter and gases (such as sulfur dioxide and nitrogen oxides) is relative humidity. Fine particles (0.1 to 2.5 microns) come from the combustion of fossil fuels and, at times, from volcanic and geological activity.

Coarse particles (2.5 to 15 microns) are typically formed as a result of human activity or originate from soil. In electronic devices, coarse particles may cause malfunctions by interrupting electrical contact between mating pairs of contacts on connectors or relays. They typically require higher relative humidity conditions than the fine particles.

According to the ISA – Instrument Systems and Automation Society standard (ISA S71.04 1985), there are four classes of industrial atmospheres with respect to copper reactivity.

	G1 (mild)	G2 (moderate)	G3 (harsh)	G4 (severe)
Copper corrosion	< 30 nm/month	< 100 nm/month	< 200 nm/month	< 300 nm/month

## Gas contaminants (ppb)

ISA category	G1	G2	G3	Gx
H <sub>2</sub> S	< 3	< 10	<50	> 50
SO <sub>2</sub> , SO <sub>3</sub>	< 10	< 100	< 300	> 300
Cl <sub>2</sub>	< 1	< 2	< 10	> 100
NO <sub>x</sub>	< 50	< 125	< 1250	> 1250
HF	< 1	< 2	< 10	> 10
NH <sub>3</sub>	< 500	< 1000	< 25000	> 25000
O <sub>3</sub>	< 2	< 25	< 100	> 100

**Table: 3.1 Airborne contaminants in gaseous molecules**

## 3.5. Forms of Corrosion

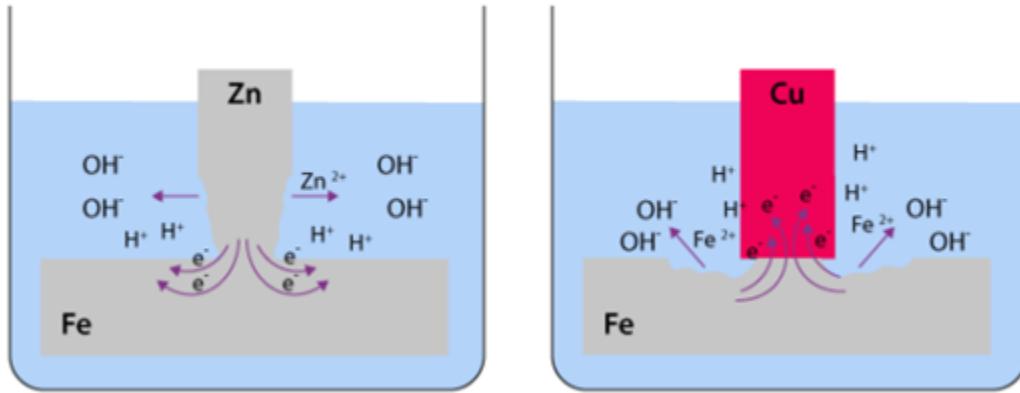
### 3.5. 1. Anodic corrosion (Galvanic corrosion)

Galvanic corrosion (also called bimetallic corrosion or dissimilar metal corrosion) is an electrochemical process in which one metal corrodes preferentially when it is in electrical contact with another, in the presence of an electrolyte.

When two metal electrodes are placed in an electrolyte and the circuit is completed by joining the metal through a wire then this is the point where the process of corrosion takes place. Metals with the higher oxidation potential will start acting as anode and will keep losing electrons whereas the metals with lower oxidation potential will start acting as cathode respectively. The activity of the metals is based on the electrochemical series. Thus the flow of current is from more active metal (anode) to less active metal (cathode).

Example, if aluminium and carbon steel are connected and immersed in seawater, the aluminium will corrode more quickly, whilst the steel will receive protection.

## GALVANIC CORROSION



**Fig: 3.9 Galvanic corrosion**

**Zinc as anode and copper as cathode :** When zinc and copper metal are placed in an electrolyte which can be of water/aqueous solution containing any salt like copper sulfate it then the circuit gets completed. Now Zinc starts to oxidize due to its high oxidation potential compared to the cathode. Thus zinc slowly starts to corrode and form zinc ions. Copper ions, on the other hand, start to gain electrons and are reduced so it is protected. The process continues until the zinc electrode entirely gets dissolved. The hydrogen ions present in the electrolyte also gets reduced to hydrogen gas and is seen as bubbles at the cathode.figure (3.9)



Galvanic corrosion can be prevented by:

1. Selecting materials with similar corrosion potentials.
2. Breaking the electrical connection by insulating the two metals from each other.

3. Applying coatings to both materials.
4. Separating the two materials by inserting a suitably sized spacer.

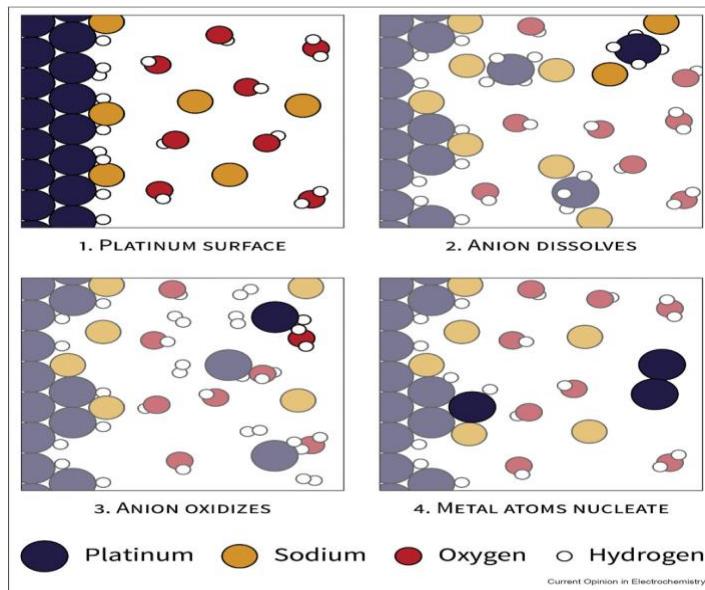
### 3.5.2 Cathodic corrosion

Cathodic corrosion is an enigmatic electrochemical process that etches metallic electrodes at potentials below 0 V *versus* the normal hydrogen electrode.

Recent advances involve applications of cathodic corrosion for nanoparticle synthesis and electrocatalyst modification. Cathodic corrosion can produce milligrams of nanoparticles in minutes or hours, using a simple voltage source and without requiring capping agents that might affect catalytic performance

#### Mechanism of cathodic corrosion

From a fundamental perspective, cathodic corrosion proceeds through the mechanism illustrated for platinum in fig 3.10 panel 1 visualizes the starting state of cathodic corrosion: a Pt surface in an NaOH solution, polarized below 0 V *vs.* the reversible hydrogen electrode (RHE). Under these conditions, Pt vigorously evolves hydrogen gas and is covered with adsorbed hydrogen atoms . A partial monolayer of  $\text{Na}^+$  is likely adsorbed as well . In these circumstances, an unknown and presumably anionic species dissolves into the working solution (panel 2). Although the identity of this species is unknown, it is likely cation-stabilized because a nonprotic electrolyte cation is required to enable cathodic corrosion . After its formation, the cation-stabilized anion moves away from the Pt surface until it encounters a water molecule (panel 3). In this encounter, the water is reduced to  $\text{H}_2$  and  $\text{OH}^-$ , whereas the anion is oxidized back to neutral platinum. These Pt atoms can then redeposit onto their native surface or nucleate in solution into nanoparticles (panel 4).



**Fig 3.10 Mechanism of Cathodic corrosion**

### 3.5.3 Electrical contact

Electrical contacts are present in any system in which a transfer of electricity occurs.

Specific examples include circuit breakers, relays, switches, and electrical discharge machining (EDM) applications.

Electrical contacts can get oxidized or corroded through the presence of moisture and oxygen. Depending on the facility, electrical connections may prematurely degrade due to high pressure, high temperatures or harsh chemicals

Production processes themselves often leave behind sources of contamination for the electrical contact surfaces, such as the solder on the circuit board surface

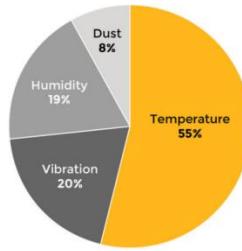
### 3.5.4. Metallic joint Degradation

#### 3.5.4.1 Factors that causes degradation of metallic joints

In electronic devices, metallic joints can also degrade due to various factors, such as:

- 1) **Thermal cycling:** Rapid temperature changes in electronic devices can cause joints to expand and contract which can lead to joint failure.
- 2) **Vibration and shock:** Electronic devices can be exposed to vibration and shock, which can cause joints to loosen or break.

- 3) **Humidity:** Moisture and other environmental factors can cause corrosion in metallic joints, which can weaken or break the joint.
  - 4) **Electrical stress:** High currents or voltage spikes in electronic devices can cause metallic joints to heat up and degrade over time.
  - 5) **Material fatigue:** Repeated stress on metallic joints can cause them to weaken and eventually fail, especially in devices that are subject to constant use or movement
- (fig 3.10)



**Fig 3.10 Chances of Metallic Joint Degradation due to various factors**

#### 3.5.4.2 Prevention

- 1) Use high-quality materials
- 2) Design the joints with the intended operating conditions in mind.
- 3) Regular maintenance and inspections to detect any signs of wear or corrosion.
- 4) Proper installation techniques and adequate stress relief measures also help to prevent joint degradation in electronic devices.

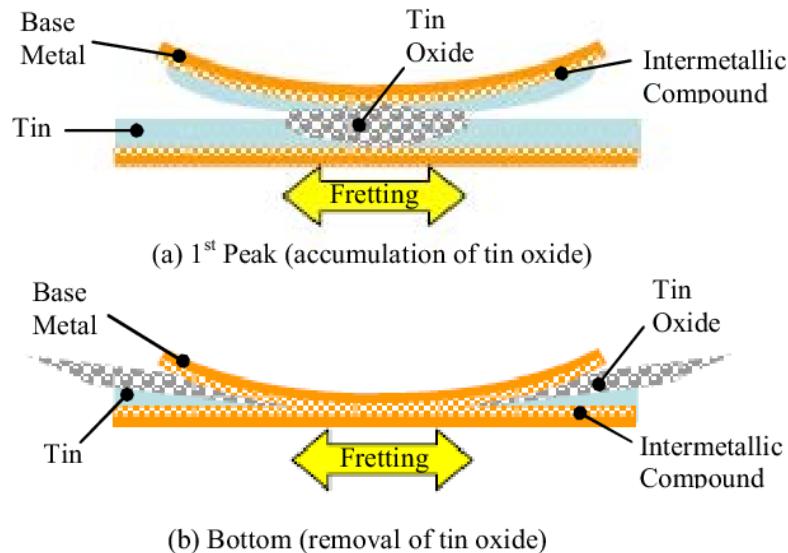
#### 3.5.5 FRETTING CORROSION

Fretting corrosion occurs due to vibration and slip in contact areas between materials under load. It appears as pits or grooves surrounded by corrosion products. fretting corrosion is also known as chafing corrosion.

Electronic devices that experience cyclic vibrations or thermal variations are susceptible to fretting corrosion

Explanation : Fretting corrosion is a common failure mechanism for tin plated copper electrical contacts. The accumulation of oxidation products at the contact spot is caused by the micro-

motions of the contact. Tin is a soft metal and rapidly forms a thin and hard oxide. When the hard oxide layer gets broken, it can be pressed into the soft and ductile tin matrix where it can accumulate. It has been speculated that it is the micro-slip action between the contacts that creates the fretting, which combined with the oxidation causes the thick insulating layer at the contact interface and the substantial increase in contact resistance and ultimate failure of the contact in figure 3.11



**Fig 3.11 Fretting corrosion in tin plated copper electrical contacts**

#### **Prevention of fretting corrosion :**

- 1) Fretting corrosion may be controlled by applying lubricants which reduce friction between the surfaces. Grease is normally used.
- 2) Use of seals to absorb vibrations and exclude oxygen and/or moisture
- 3) Increase the hardness of one or both materials in contact.

### **3.6. Corrosion cost**

#### **3.6.1 Introduction**

- 1) Corrosion is a significant issue in India, with direct and indirect costs affecting various sectors of the economy. According to a study conducted by the National Association of Corrosion

Engineers (NACE), the cost of corrosion in India is estimated to be around 3-6% of the country's GDP (gross domestic product )

2) Analysis of 26 industrial sectors, in which corrosion is known to exist, and extrapolating the results for a nationwide estimate ,it is investigated that the annual corrosion costs ranged from approximately 1 to 5 percent of the Gross National Product (GNP) of each nation.

### **3.6.2 Various sectors affected by Corrosion**

#### **1) Infrastructure**

Infrastructure is particularly vulnerable to corrosion, with structures like bridges, roads, and pipelines experiencing significant damage due to corrosion. The cost of maintaining and repairing corroded infrastructure is high.

#### **2) Transportation sector**

The transportation sector is also impacted by corrosion, with vehicles, railways, and shipping experiencing significant wear and tear due to corrosion. This can lead to increased maintenance costs and reduced efficiency.

#### **3) Oil and gas sector**

The oil and gas sector is particularly susceptible to corrosion, with pipelines and equipment experiencing significant damage due to corrosive substances. The cost of repairing or replacing corroded equipment is high, and corrosion-related accidents can be dangerous.

#### **4) Power sector**

The power sector is also impacted by corrosion, with power plants and transmission lines experiencing significant damage due to corrosion. This can lead to reduced efficiency and increased maintenance costs.

#### **5) Manufacturing sector**

The manufacturing sector is impacted by corrosion, with equipment and machinery experiencing significant wear and tear due to corrosion. This can lead to increased maintenance costs and reduced productivity.

Overall, the cost of corrosion in India is significant and has a wide-ranging impact on various sectors of the economy.

### **3.6.3 Reducing corrosion cost**

Addressing the issue of corrosion is crucial for the sustainable growth and development of the country. The cost of corrosion can be reduced through the use of corrosion-resistant materials, regular maintenance and inspections, and proper training and education for workers.

## **3.7. Corrosion protection of computer hardware**

Corrosion protection is essential for computer hardware, as corrosion can damage or destroy components, leading to costly repairs or replacements.

It requires a combination of proper storage, maintenance, and protection measures. By taking these steps, computer hardware can be protected from corrosion damage and have a longer lifespan.

Computer hardware refers to the physical components of a computer system that can be touched, seen, and manipulated.

### **3.7.1 Components of computer hardware**

**Central Processing Unit (CPU):** The CPU is the brain of the computer that performs all the processing tasks. It is a microchip that interprets and executes instructions.

**Motherboard:** The motherboard is the main circuit board that connects all the other components of the computer, such as the CPU, memory, and storage.

**Memory:** Memory refers to the computer's temporary storage that is used to store data that the CPU needs to access quickly. The two main types of memory are Random Access Memory (RAM) and Read-Only Memory (ROM).

**Storage:** Storage refers to the long-term memory of the computer that is used to store data and software programs. The two main types of storage are Hard Disk Drives (HDD) and Solid State Drives (SSD).

**Input devices:** Input devices are used to enter data into the computer system. Examples include keyboards, mice, scanners, and microphones

**Output devices:** Output devices are used to display or output data from the computer. Examples include monitors, printers, and speakers.

**Peripheral devices:** Peripheral devices are hardware components that connect to the computer system, such as external hard drives, webcams, and USB drives.

### **3.7.2 Measures to protect computer hardware**

#### **1) Dust and Debris**

Keep the computer hardware clean and dry. Regular cleaning with a soft, dry cloth can remove dust and debris that can cause corrosion.

#### **2) Temperatures and Humidity Protection**

Avoid exposure to extreme temperatures and humidity. Store computer hardware in a cool, dry place away from direct sunlight, and avoid placing it near heat sources like radiators or vents.

#### **3) Moisture Protection**

Use protective covers or cases for laptops and other portable devices when not in use. This can help prevent exposure to moisture and other environmental elements that can cause corrosion.

Use desiccants, such as silica gel packets, to absorb moisture in storage areas or during transport. This can help prevent moisture damage to computer hardware.

#### **4) Corrosion-resistant materials**

Use corrosion-resistant materials for computer hardware components. This can include using stainless steel or aluminum for cases and other metal components.

Apply protective coatings or treatments, such as a corrosion-resistant spray, to computer hardware components. This can help prevent corrosion damage.

#### **5) Regular inspection**

Regularly inspect computer hardware for signs of corrosion or damage. Early detection and treatment can prevent further damage and costly repairs or replacements.

## **SELF ASSESSMENT**

### **PART-A**

1. How does corrosion affect electrical systems?
  - a) It causes more than 50% of electrical system downtime
  - b) It enhances the performance of controls and switching gear
  - c) It results in the strengthening of metallic wire terminals
  - d) It has no effect on electrical systems
2. What is the impact of increased use of electronics on corrosion reliability?
  - a) It has no impact
  - b) It has decreased the demand for corrosion reliability
  - c) It has increased the demand for corrosion reliability
  - d) It has made corrosion reliability irrelevant
3. Select the cause of corrosion in metallic wire terminals.
  - a) Physical deterioration
  - b) Chemical attack
  - c) Electrochemical deterioration
  - d) All of the above
4. What is the main concern for industrial electronics?
  - a) Lifetime performance
  - b) Aesthetics
  - c) Cost-effectiveness
  - d) Reliability
5. Recall the material used as the substrate in epitaxial growth
  - a) P-type silicon
  - b) N-type silicon
  - c) Germanium
  - d) Carbon
6. What is the purpose of vias in a PCB?
  - a) A. To provide a place to connect components to the board
  - b) To make the board more visually appealing
  - c) To electrically and thermally join polygons on different layers of a PCB
  - d) To hold the components in place on the board

7. Select the G3 class limit according to the ISA with respect to copper activity.

- a) >200nm/month
- b) <300nm/month
- c) <200nm/month
- d) >50nm/month

### **Part-B**

Discuss the corrosion due to miniaturization of electronic devices.

Summarize the chafing corrosion in electronic device.

Predict the salient features of Epitaxial Process.

Interpret the various parts of Printed Circuit Board.

List the general causes of corrosion in electronic devices.

### **Part- C**

Describe the various steps involved in fabrication of Integrated Circuit chip.

Paraphrase the major forms of corrosion observed in electronic systems.

Explain the corrosion protection of computer hardware with its components.

Enumerate the chemistry involved in the manufacture of Printed Circuit Board.

Illustrate the causes of corrosion due to environmental contamination ,production and service factors

**UNIT:1V**  
**COMPUTATIONAL CHEMISTRY**

**4.1: INTRODUCTION**

Computational chemistry has emerged as an applied branch of Chemistry that involves multidisciplinary knowledge, connecting related fields such as chemistry, computer science, biology, pharmacology, physics, and mathematical statistics.

The computational chemistry can be termed as applied form of theoretical chemistry. The results of theoretical chemistry are incorporated into a computer program to calculate the optimised structure and henceforth the properties of molecules.

As an example, pharmacy companies synthesize thousands of chemical compounds every year to understand the molecular structure of the compounds and its effect in patients. Modifying any chemical reaction is expensive. Usage of the computer models narrow down the search. This can be done by designing drugs through computer models and check its reactivity with biomolecules. Only those chemicals which are expected to give useful results can be experimentally synthesized and taken further for real time research.

**4.2: Software tools available for chemistry and its applications**

**Molecular modeling software**

**(i)ChemDoodle**

ChemDoodle is a chemical sketcher that contains many features for working with chemical graphics. This molecular modeling software for chemistry is one of the best you can find on the market. It has a very user-friendly UI (Users Interface) which can be used by school students to chemical engineers. It can create chemical 3D structures with high-quality 3D graphics and quickly build and manage reaction schemes in real-time.

ChemDoodle comes with some software tools, called “Widgets”. These are mini-applications that perform various tasks to contribute to the creation of molecular graphics. Such tasks may be the calculation of molecular masses, conduction of elemental analysis, search of databases for chemical structures, etc. Moreover, ChemDoodle includes a visualization platform, called ChemDoodle 3D, that turns the 2D chemical structures into customized 3D models.

The software is compatible with Windows, Mac OS X, and Linux. It is also available on smartphones, which allows transferring your 3D designs between desktop and mobile.

#### **(ii) Hypercube**

Hypercube is a molecular modeling software that is used by many chemists for its functionality and user-friendly UI (Users Interface). The main package of this molecular design software is “HyperChem”. “HyperChem” software supports many functions related to chemistry 3D design, such as protein simulations, molecular modeling, molecular visualization, calculations of chemical structures and other operations related to bioinformatics.

Hypercube offers various other specialised molecular modeling software, depending on your field of activity in chemistry. One of them is “HyperProtein” software, which focuses on the modeling of proteins. Apart from the main features related to modeling and simulation that HyperChem software can provide, it includes some software related to sequence alignment and phylogenetic tree creation for families of proteins.

#### **(iii) Avogadro**

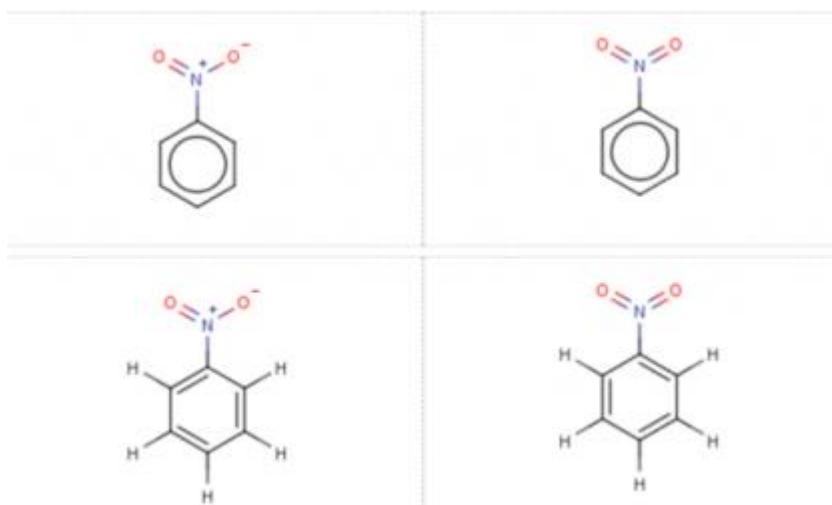
Another molecular modeling software for chemistry you may find easy to use is Avogadro.

Avogadro is a software which supports the import of chemical files and generates multiple computational chemistry packages. It is used in many fields of scientific activity, such as computational chemistry, molecular modeling bioinformatics and materials science, from students to experienced chemists. One of the key advantages of this software is that it offers flexible high-quality rendering and advanced features for molecule editing.

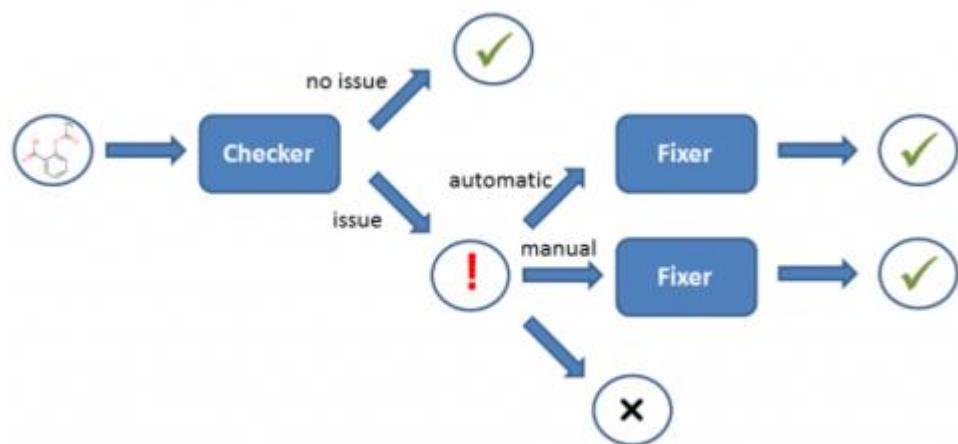
#### **(iv) ChemAxon**

ChemAxon is a chemical structure representation toolkit that you may find very useful if you are a chemical engineer or even an undergraduate student in chemistry. The software has two main features, which are located in two individual applications. The first one of these features is called “Standardizer”, and helps you to turn your chemical structures into customized 3D

molecular representations. Apart from the many predefined actions that the application provides, the user can implement some of his own. The other key feature of this design software for chemistry is called “Structure Checker”. This application offers you the possibility to edit and modify any issues you may have with the structure of the molecular drawing. It searches the molecules for structural problems and once an error is found, the software provides automatically a real-time solution. “Structure Checker” is a very useful tool that any user of chemical drawing will appreciate, as it spots errors and incorrect features, especially when a new molecule is added to the drawing space.



“Standardizer” feature – [chemaxon](#)



“Structure Checker” feature – [chemaxon](#)

#### **(v) BIOVIA Draw**

BIOVIA Draw is a molecular drawing software that is addressed mainly to chemists and experienced professionals of the chemical industry. It offers scientists a complete set of tools for drawing and modifying complex molecules, chemical reactions and biological sequences. Its interface is easy to learn, and offers the possibility of viewing, communicating, and archiving of scientific information.

#### **(vi) MolView**

MolView is a modeling software for chemistry with a quite different interface than the other packages mentioned above. Its main difference consists in the fact that it is a free and online web-application. It is a very easy program to use, even if you have no prior experience in kind of 3D modeling software. This Open-Source web-application can be used both as molecular editor and as a 3D model viewer. As a user, you are allowed to upload molecules from large databases like PubChem, RCSB Protein Data Bank and the Crystallography Open Database. With MolView, apart from creating structural formulas, you can also use it for protein display, modeling and simulation of proteins assembly and Chain representation. Last but not least, you can also export different kinds of data in PNG format (as snapshot from interactive spectrum) or in JCAMP file format (JCAMP-DX file of the current spectrum).

#### **(vii) ACD/ChemSketch**

ACD/ChemSketch is chemical drawing package that you can either download for free or purchase if you aim to use it for commercial purposes. But keep in mind that the free version of ChemSketch does not include all the features of the commercial version. However, it is a pretty complete software that can be used for educational purposes, either by high school students or by undergraduate chemistry students. With this software, you can draw organic chemical structures, structures of organometallics, polymers and Markush structures. As a user, you are also given the possibility of calculating molecular properties, such as molecular weight, density, molar refractivity etc. It is also possible to preview your 2D molecular design in 3D to visualize better the designed structure.

#### **(viii) ChemDraw**

**ChemDraw** is a molecule editor first developed in 1985 by David A. Evans and Stewart Rubenstein (later by the cheminformatics company CambridgeSoft). ChemDraw

Professional is a drawing tool that allows users to **draw chemical structures and reactions as well as biological objects and pathways**. Users can also use it to predict properties and spectra, convert chemical structures to IUPAC names, view 3D structures, etc.

### **Features of ChemDraw 12.0**

- a) Chemical structure to name conversion.
- b) Chemical name to structure conversion.
- c) NMR spectrum simulation ( $^1\text{H}$  and  $^{13}\text{C}$ )
- d) Mass spectrum simulation.
- e) Structure cleanup.
- f) Draw ligand Structure.
- g) An extensive collection of templates, including style templates for most major chemical journals.
- h) Export to SVG.

### **(ix) Gaussian**

**Gaussian** is a computer program used by chemists, chemical engineers, biochemists, physicists and other scientists. It utilizes fundamental laws of quantum mechanics to predict energies, molecular structures, spectroscopic data (NMR, IR, UV, etc) and much more advanced calculations. It is released in 1970 by John Pople and his research group at Carnegie-Mellon University as Gaussian 70. It has been continuously updated since then and **Gaussian09** is the latest version in the Gaussian series of programs. It provides state-of-the-art capabilities for electronic structure modeling. Gaussian09 is licensed for a wide variety of computer systems.

### **Gauss view**

**GaussView** is a graphical user interface designed to help you prepare input for submission to Gaussian and to examine graphically the output that Gaussian produces. GaussView is not integrated with the computational module of Gaussian, but rather is a front-end/back-end processor to aid in the use of Gaussian. GaussView provides three main benefits to Gaussian users.

- 1) GaussView offers you an advanced visualization facility.
- 2) GaussView makes it easy to set up many types of Gaussian calculations.
- 3) GaussView lets you examine the results of Gaussian calculations using a variety of graphical techniques.

## **4.3: Chem Draw- Designing a Chemical Structure**

### **4.3.1: The Main Tools Palette**

Use the main tools palette to create and manipulate drawings. The appearance of the toolbar is slightly different for the different versions of ChemDraw. The toolbar for ChemDraw Ultra is shown below.

The table below describes the functions of the tools for all versions. Some of the tools have multiple options that can be selected from a tool palette.

Tool	Use to...
Selection	Lasso-select objects by dragging around them. Marquee-select objects by dragging diagonally across them. Selected objects can be further manipulated using menu commands.
Structure Perspective	Rotate a selected object in three dimensions.
Mass Fragmentation tool	Splits molecules across specific bonds.
Bond	Draw bonds and set bond properties.
Eraser	Delete objects. Click on an object to delete; drag to delete multiple objects.
Multiple Bonds	Draw multiple bonds and set bond properties. Bonds of different types can be selected from the Multiple Bonds tool palette.
Text	Create atom labels and captions.
Pen	Draw freehand shapes such as custom arrows and orbitals.
Arrow	Draw arrows. Arrows of different types can be selected from the Arrows tool palette.
Orbital	Draw orbitals. Orbitals of different types can be selected from the Orbitals tool palette.
Drawing Elements	Draw annotations that lack chemical significance, such as boxes and lines. Drawing Elements of different types can be selected from the Drawing Elements tool palette.  Includes the Arc tools.
Brackets	Draw brackets, parentheses, and braces. Brackets of different types can be selected from the Brackets tool palette.
Chemical Symbols	Draw chemically significant symbols such as charges, radicals, and lone pairs. Symbols of different types can be selected from the Symbols tool palette.
Arc	Draw arcs. Arcs of different degrees can be selected from the Arcs tool palette. <i>NOTE: The Arcs tool is a separate tool only on ChemDraw Standard.</i>
Acyclic Chain	Draw chains of any length.
Query Tools	Draw stereochemical flags, indicate free sites, alternative groups and correspondences between atoms in query structures. Various options can be

	selected from the Query tool palette.
Templates	Draw structures with templates stored in template documents. Templates can be selected from the Templates tool palette.
Rings	Draw common structural components.
Table	Draw tables with multiple rows and columns.
TLC Plate	Draw TLC plates with multiple lanes and adjustable solvent front and spots.

#### **4.3.2:** Compile Chemdraw and Gaussian molecular modelling software tools .

Hotkeys are organized into atom labels, bond types, and functions (such as adding a charge or displaying a bond). Shortcuts are organized by the menu on which the command is found.

Atom Keys Use atom keys to insert atoms in a drawing using your keyboard. For example, place your mouse over an atom and press <3>to add a tert-butyl group.

ATOM LABEL	KEY
A	a
F	f
Ph	P or 4
Ac	A or 5
H	h
Q*	q
Br	b
I	i
R	r
n-Bu	l
K	k
S	s
s-Bu	2
Me	m

TMS	t
-----	---

#### **4.3.3: Bond Hotkeys**

To modify a bond, place your mouse over the bond and select a key listed below.

Function	Key
Change to single bond	1
Change to dashed bond	d
Change to double bond	2
Change to wavy Bond	y
Change to triple Bond	3
Position a double bond to the left	I
Change to quadruple Bond	4
Center a double Bond	c
Change to bold Bond	b

#### **4.3.4: Function Hotkeys**

To apply function hotkeys, place your mouse over an atom and press the appropriate key.

Function	Key
Add an attachment point	. (period)
Add an atom number	' (single quote)
Add a negative charge	-
Add a positive charge	+
Sprout one bond	0
Sprout two bonds	9
Sprout three bonds	8

Display the Atom Properties dialog box	/ (slash) or ?
Display the Choose Nickname dia-	= (equals)

### **4.3.5: Shortcuts**

Below is a list of key combinations for common tasks.

#### **4.3.5.1: View commands and structure commands**

##### **View**

Command	Key Combination
Actual size	F5
Reduce	F8
Magnify	F7
Fit to window	F6
Toggle ruler	F11
Toggle crosshair	CTRL

##### **Structure**

Command Key	Combination
Clean up structure	SHIFT+CTRL+K
Convert name to structure	SHIFT+CTRL+N
Convert structure to name	ALT+CTRL+N

#### **4.3.5.2: View Commands**

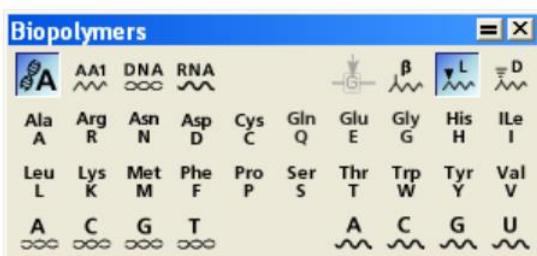
Enter	To execute command
F5	Actual size
F8	Reduce
F7	Magnify
F6	Fit to window

F11	Toggle ruler
CTRL	Toggle crosshair

#### 4.3.5.3: Object Commands

Enter	To execute command
F2	Bring to front
F3	Send to back
Ctrl+E	Toggle fixed angles
Ctrl+G	Group selected objects
Shift+Ctrl+G	Ungroup objects
Shift+Ctrl+H	Flip horizontal
Alt+Shift+H	Rotate 180° horizontal
Ctrl+J	Join selected objects

#### 4.4: Biopolymers Drawing



The Biopolymers toolbar includes the following options:

**Biopolymer Editor:** Enables all the nucleic and amino acids

**Single Letter Amino Acid:** Enables all the amino acids

**Beta Amino Acids, L-Amino Acids, D-amino Acids:** Enables addition of Beta, L-, and D-

**DNA Sequence:** Enables the deoxyribonucleotides that can be used to create a DNA molecule

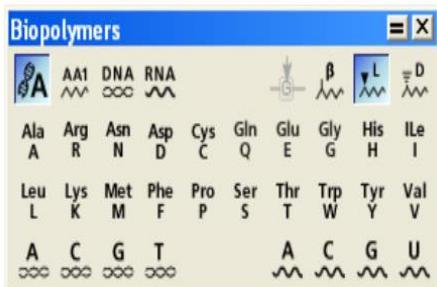
**RNA Sequence:** Enables the ribonucleotides that can be used to create a RNA molecule

**To draw a sequence:**

1. Select one of these tools from the Biopolymer toolbar
2. Click where you want to start the sequence. A text box appears.
3. In the text box, enter the single-letter label for the residue.
4. Repeat step 2 for each residue.
5. When your chain is complete, press , or <Esc>

#### **4.4.1: Biopolymer Editor**

The Biopolymers toolbar contains a tool called Biopolymer Editor.



Using the biopolymer editor, you can create a sequence by explicitly specifying the residue name instead of the IUPAC code. For example, when you enter 'a', the residue 'Ala' is suggested. To accept the suggestion, press or key. Press TAB to move the caret to the end of the selected label. To enter b amino acids, type a nickname such as bAla. The 'b' is converted to the b symbol. You can also create b amino acids using the b- amino acid button in the biopolymer editor. b- amino acids always display using three-letter codes. Glycine does not have a beta carbon, and so there is no beta version.

#### **4.5: Advanced drawing Techniques**

It includes two features for generating structures and chemical names—Name>Struct and Struct>Name. Collectively, these features are called Struct=Name

Struct>Name generates the names of chemical structures using the Cahn-Ingold-Prelog rules for stereochemistry. Using this option, you can generate the name of structures you have drawn.

Name>Struct lets you convert chemical names into their corresponding chemical structures. It is designed to interpret chemical names as they are used by chemists. In other words, it recognizes the shorthand and slang of everyday usage, in addition to recognizing most of the official IUPAC, IUBMB, and CAS rules and recommendations.

#### **4.5.1: Struct>Name**

Struct>Name can interpret a variety of chemical structures. This means that you can draw a structure and Struct>Name will provide its name. It also updates the name when you modify the structure.

##### Using Struct>Name

To generate the name of your structure:

1. Select the structure.
2. Navigate to Structure>Convert Structure to Name. The name appears under the structure.

#### **4.5.2: Name>Struct**

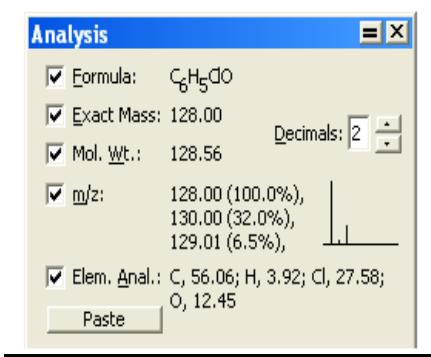
##### Converting Names to Structures

To enter the name and convert it to its structure:

1. Navigate to Structure>Convert Name to Structure. The Insert Structure dialog box appears.
2. Type the name (example: 2-bromobenzoic acid) or paste the copied name from the clipboard.
3. To place the name below the structure, select Paste name below structure.
4. Click OK.

#### **4.5.3: Structure Analysis**

Using the analysis window, chemical formula, exact mass, molecular weight, m/z, and elemental analysis for the entire document, a structure, or a part of a structure can be displayed.



The Decimals setting applies to Exact Mass, Molecular Weight, and m/z only. The values displayed in the Analysis window includes:

**Formula:** The molecular formula showing the exact number of atoms of each element in the molecule and charges, radicals, and isotopes.

**Exact Mass:** The exact molecular mass of the structure, where atomic masses of each atom are based on the most common isotope for the element.

**Molecular Weight:** The average molecular mass of the structure, where atomic masses are based on the natural abundance of all isotopes of the element.

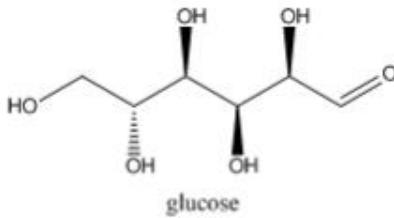
**m/z.Mass/charge:** The weights of the most common isotopes and a graphical representation of the isotopic abundance is shown.

The molecular weight accounts for the isotopes for each atom and their natural abundance. Where there is more than one abundant isotope, this feature computes multiple molecular weights. Low abundance combinations (whether because the isotope is in low abundance or because it includes many moderate-abundance contributions) are not taken into account.

#### 4.5.4: Elemental Analysis

The percent by weight of each element in the structure. To open the analysis window:

1. Select the entire structure, or part of the structure. If nothing is selected, the analysis window displays value for the entire structure.
2. Navigate to View>Show Analysis Window. The analysis windows displays values for the parts of the drawing you select, or the entire drawing if nothing is selected.
3. (Optional) Select Paste to add the analysis information to your drawing. The information appears as a caption that you can edit.



Chemical Formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>

Exact Mass: 180.06

Molecular Weight: 180.16

m/z: 180.06 (100.0%), 181.07 (6.9%), 182.07 (1.4%)

Elemental Analysis: C, 40.00; H, 6.71; O, 53.29

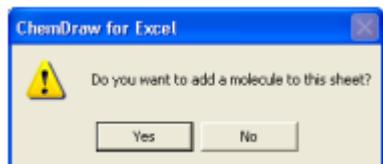
#### **4.5.5: Adding Structures with ChemDraw**

The most direct way to insert a new structure into a cell is by using ChemDraw.

To add a structure with ChemDraw:

1. Double-click in a cell.

The ChemDraw/Excel dialog box appears:



2. Click Yes. ChemDraw opens.
3. Draw the structure in ChemDraw.
4. From the ChemDraw File menu, click Close and Return to New Molecule. The new structure appears in the cell.

#### **4.6: Creating 3D Models**

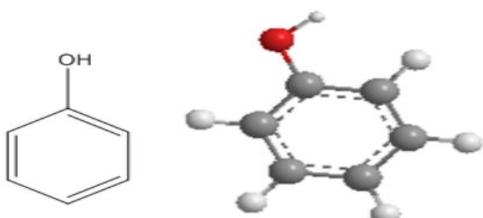
As you create your drawing, you can view it in three-dimensions.

Two features in ChemDraw let you view structures in three dimensions.

#### **3D Model**

Use a 3D model to paste a 3D version of the structure into your drawing.

1. Select the structure.
2. Navigate to Edit>Get 3D Model. The 3D structure appears in the document window.



To view the model in Chem3D, double-click on it.

## Chem3D Preview Options

The preview window displays structures you select in 3D and displays all structures if none are selected.

Chem3D Preview works only for chemical structures.

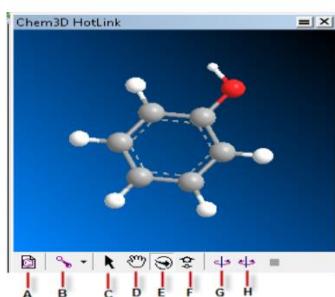
### In the Document Window

With the preview window open, you can still change your drawing in the document window.

The preview window updates to reflect the changes.

### In Chem3D Preview

The preview window offers several options to view structures.



## Launch Chem 3D

The structure will appear in Chem3D as a model that you can edit.

**Display Mode.** Choose display options for the model: wire frame, stick, ball & stick, cylindrical bonds, and space filling.

**Select:** Select the structure or parts of it.

**Translate:**Move the structure.

**Rotate:**Rotate the structure in three dimensions (the image rotates only in the Chem3D Preview).

**Zoom:**Enlarge or reduce the apparent size of the structure.

**Spin:**Rotate the structure horizontally in one direction.

**Rock:**Rotate the structure horizontally back and forth.

## Returning to the Document Window

To exit the Chem3D Preview, close the preview window.

### To edit the 3D model:

1. Double-click the 3D structure. Chem3D opens.
2. Edit the structure and close Chem3D. The edited structure appears in the ChemDraw document window.

## 4.7: Estimating & displaying proton and $^{13}\text{C}$ NMR Chemical Shifts

### 4.7.1: NMR Shifts

Chem NMR estimates chemical shifts for all hydrogen or carbon atoms for which additivity rules are available.

Following a hierarchical list, it first identifies key substructures of a molecule. A substructure provides the base value for the estimated shift. For example, benzene would be the key substructure of trinitrotoluene. When a substructure is a ring system not available in the data, Chem NMR approximates its base shift using embedded rings and, if necessary, will disassemble the ring into acyclic substructures.

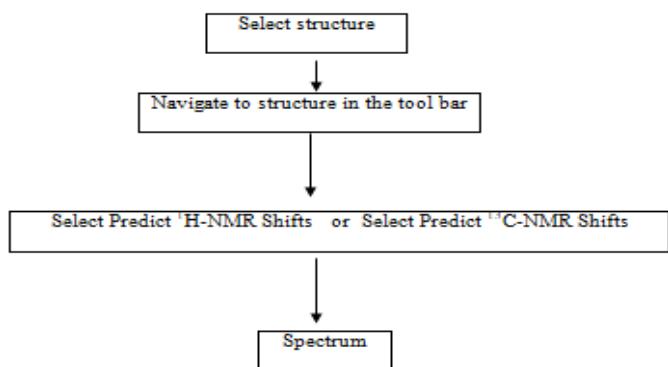
ChemNMR views remaining parts of the molecule as substituents of a substructure. Each substituent adds to, or subtracts from, the base shift of the substructure to which it is attached. Additivity rules determine the increment of each contribution. If an increment for a substituent cannot be determined, ChemNMR uses embedded substituents—smaller structural units with the same neighboring atoms. Or, it will use increments of identical, or embedded substituents, of a corresponding substructure by assuming that the effects of the substituents are of the same magnitude. ChemNMR provides a detailed protocol of the estimation process applied. It gives substructures as names, compound classes in most cases,

substituents in the form of a linear code, respectively. It also implements models for ethylenes (cis/trans) and cyclohexanes (equatorial/axial)

#### **4.7.2: To view $^1\text{H}$ or $^{13}\text{C}$ NMR information:**

1. Select a structure.
2. Navigate to Structure>Predict  $^1\text{H}$ -NMR Shifts or Predict  $^{13}\text{C}$ -NMR Shifts.

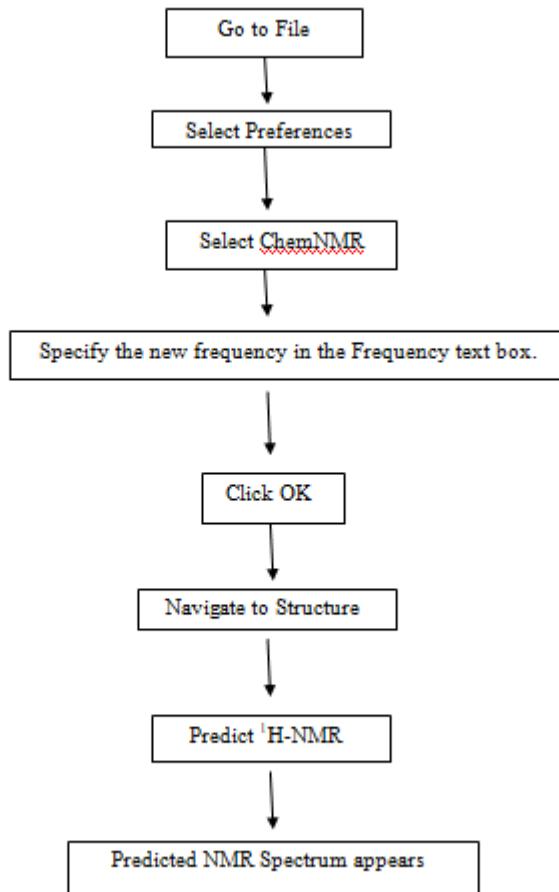
ChemNMR redraws the molecule with the estimated shifts and displays the information and line spectrum in a new window.



#### **4.7.3: Modifying NMR Frequency**

##### **To change the frequency:**

1. Navigate to File>Preferences. The Preferences dialog appears.
2. Select ChemNMR option.
3. Specify the new frequency in the Frequency text box.
4. Click OK.
5. Navigate to Structure>Predict 1H-NMR Shifts. The predicted NMR spectrum appears.



#### **4.7.4: Assigning Structures to Spectra**

ChemDraw Professional lets you assign structures to spectra. You can then display the structure associated with a specific peak by placing the pointer on that peak.

##### **To assign structures to spectra:**

1. Open a spectral file.
2. Draw the structure (or structures) to assign to the spectrum.
3. Select specific atoms and bonds in the structure.
4. +click the peak, or peaks, to which you want the structure assigned. The selection rectangle surrounds the selected objects.
5. Navigate to Structure>Make Spectrum-Structure Assignment.

The selected atoms and bonds in the structure are associated with the selected spectral peaks.

#### **4.7.5: Viewing Spectral Assignments**

To view spectral assignments:

1. Click the Lasso or Marquee tool.
2. Place the pointer over a peak. The assigned atoms or bonds are highlighted.

#### **4.7.6: Removing Spectral Assignments**

To remove spectrum to structure assignments:

1. Click the Lasso or Marquee tool.
2. Select the objects from which to remove the assignment.
3. Navigate to Structure>Clear Spectrum-Structure.

#### **4.8: Creating TLC Plates to find R<sub>f</sub> values**

The TLC Tool is a drawing tool that allows you to easily depict Thin Layer Chromatography plates within a ChemDraw document. The tool creates a rectangular plate with origin line, solvent front, and one or more lanes. The lanes can be populated with spots of different R<sub>f</sub>, size, shape, or color.

##### **To create a TLC plate:**

1. Select the TLC tool  .
2. Drag in any direction from the point of origin.  
The number of lanes is a function of the width of the plate you create.

You can manipulate parts of the plate as follows:

If you want to...	then...
Change the height or width of the plate.	Drag a border or corner. The number of lanes will not change.
Move the origin or solvent front.	Drag the origin or solvent front line.
Change the order of lanes.	Drag the origin tick to the new location.
Add, delete or duplicate a lane.	<ol style="list-style-type: none"><li>1. Control-click in the plate.</li><li>2. Select the appropriate action.</li></ol> <b>NOTE: You can also delete lanes with the Eraser tool.</b>
Move a spot.	Drag the spot. The R <sub>f</sub> displays as you drag.
Duplicate a spot.	Option+Drag the spot.
Delete a spot.	Click on the spot with the Eraser tool. <b>NOTE: If you erase all spots in a lane, the lane will be deleted.</b>

Display the R <sub>f</sub> for a spot.	1. Control-click on a spot. 2. Select Show R <sub>f</sub> . <b>NOTE: To display R<sub>f</sub> for all spots, Control-click in the plate and select Show R<sub>f</sub> from the TLC Spots submenu.</b>
Change the style or color of a spot.	1. Control-click on a spot. 2. Choose the style or color. <b>NOTE: To change the style for all spots, Control-click in the plate and choose the style from the TLC Spots submenu.</b>
Enlarge or "smear" a spot.	<p>Shift+drag the spot. When you position the cursor on a spot and press "Shift", the cursor assumes one of three shapes, depending on how it is positioned:</p> <ol style="list-style-type: none"> <li>1. Cross arrows  -used to enlarge a spot.</li> <li>2. Horizontal arrow  -used to widen a spot.</li> <li>3. Vertical arrow  -used to elongate a spot.</li> </ol> <p><b>NOTE: You may want to zoom in to make positioning easier.</b></p>

## **4.9: Chem Draw/Excel functions**

ChemDraw/Excel allows the user to create chemically knowledgeable spreadsheets within the familiar Microsoft Excel environment. We can build and manipulate chemical structures within Excel, compute chemical properties and perform database searches.

ChemDraw includes an Excel add-in — but we have to tell Excel that you want to use it!

### **4.9.1: Method:1**

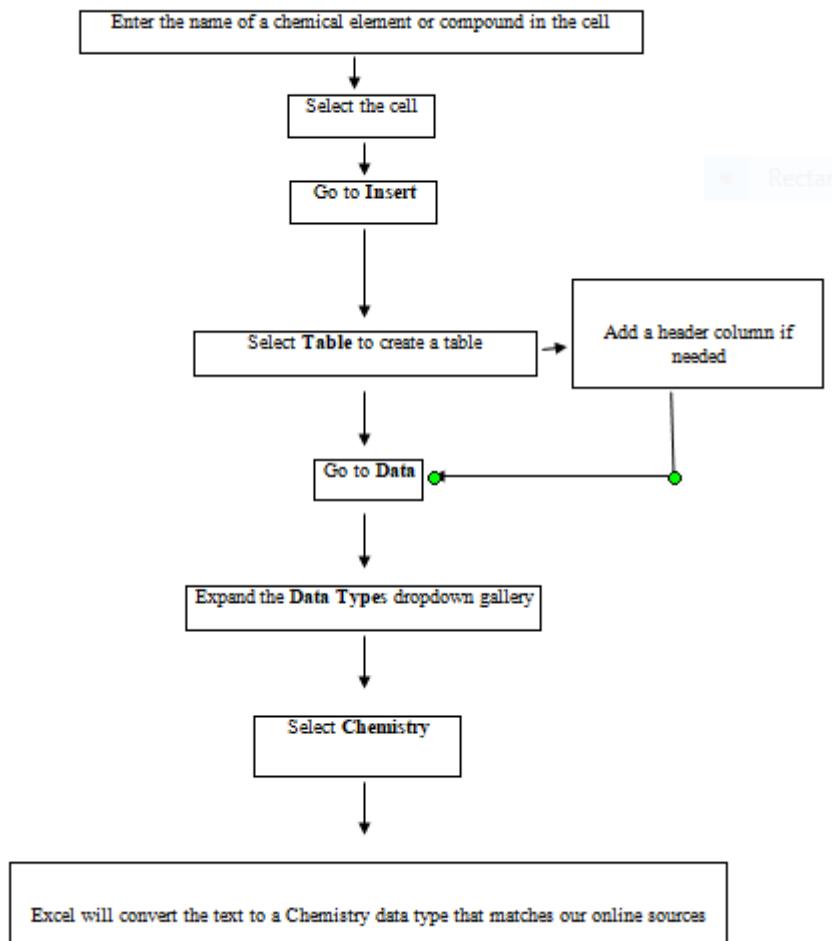
In a cell, enter the name of a chemical element, chemical compound, isotope, mineral or chemical formula. For example, you might enter “Hydrogen”, “Water”, or “H<sub>2</sub>O”. If you’re entering multiple, make sure each is in its own cell in a column.

Select these cells and go to **Insert > Table** to create a table. Add a header column if desired.

**Note:** While creating a table isn't required, we recommend putting your text in a table for the best experience.

With the table selected, go to **Data >** expand the **Data Types** dropdown gallery > select **Chemistry**.

Excel will convert the text to a Chemistry data type that matches our online sources. You'll know it's converted if the Chemistry data type icon appears in the cells.



**Note:** If you see a question mark icon in the cell, this means that Excel needs your help to clarify a match. See the section on using the Data Selector below.

To add data to your table, select one or more converted cells and the **Add Column** button will appear. Select that button and select any of the fields to add those facts to the table.

#### **4.9.2: Method:2**

On Excel's "Tools" menu, select "Add-ins" and turn on ChemOffice or ChemDraw.

In Excel, chemically-intelligent spreadsheets include a menu item like "ChemOffice11" right next to the "Window" menu.

To create chemical spreadsheets, use menu item "New ChemOffice Worksheet" instead of "File > New > Worksheet".

To identify chemical spreadsheets, the Excel worksheet name is "ChemOffice1" instead of "Sheet1".

When using chemical spreadsheets, molecular structures are embedded within cells, instead of "floating" above cells.

A new set of "ChemDraw Functions" appears on the "Insert Function" list, alongside "Financial" and "Statistical" functions.

ChemDraw Functions include chemical analysis, property predictions, molecular topology, and SMILES conversions.

#### **4.9.3: Method:3**

##### **Importing Tables**

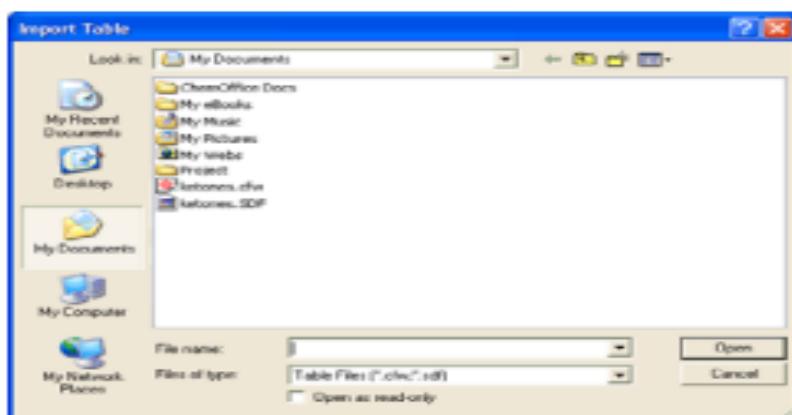
ChemDraw/Excel allows you to import from the following sources:

- MDL SDFfiles—Imports all records in the file. Each structure is given the name stored in the SDFfile.
- ChemDraw databases —Imports all fields stored in the main form. Molecular weight and formula fields are not imported because ChemDraw/Excel calculates them. Each structure is named Structure , where n is a unique number.

##### **To import a table:**

1. Select the cell where you want the import to start. The upper left corner of the import is at this cell. Data is filled down and to the right.
2. From the ChemOffice menu, select Import Table or click.

The Import Table dialog box appears.



- 3.Type or select the file name to import and click Open.

All records are added to your spreadsheet.

##### **Exporting Tables**

ChemDraw/Excel allows you to export tables to MDL SDFfiles.

Selected cells are exported to a specified file. If no cells are selected, the entire spreadsheet is exported. The first column of the area to export must have the word “Structure” in its top cell. Structures outside the first column will be discarded.

The screenshot shows a Microsoft Excel spreadsheet titled "STRUCTURE". The table has columns labeled A, B, C, D, and E. Row 1 contains the headers: STRUCTURE, MOL\_ID, FORMULA, MOLWEIGHT, and MOLNAME. Rows 2, 3, and 4 contain data for three structures: Structure1 (C10H16O, 152.2358, Camphor), Structure2 (C6H10O, 98.1444, Cyclohexanol), and Structure3 (C13H10O, 182.2214, Benzophenone).

A	B	C	D	E
1	STRUCTURE	MOL_ID	FORMULA	MOLWEIGHT
2	Structure1	1	C10H16O	152.2358
3	Structure2	2	C6H10O	98.1444
4	Structure3	3	C13H10O	182.2214
				Benzophenone

### To export data:

1. Select the information to export:

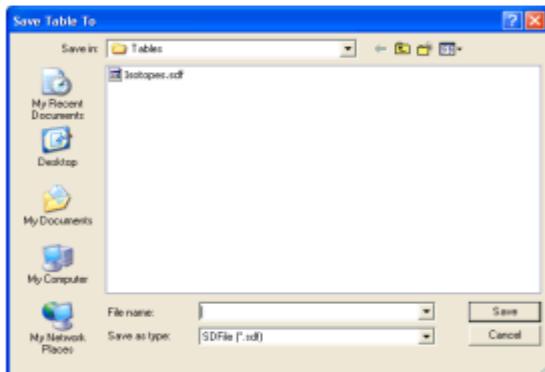
**If you want to export Then**

a specified area of your spreadsheet      Select the area to export.

the entire spreadsheet      Do not make any selection.

2. From the ChemOffice menu, select Export Table or click.

The Save Table To dialog box appears



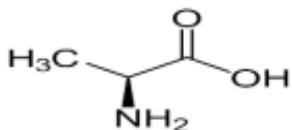
3. Type the file name and click Save. The table is saved to the specified file.

## **SELF ASSESSMENT**

### **PART-A**

- 1.What is the applied form of computational chemistry?
  - a. Theoretical chemistry
  - b. Experimental chemistry
  - c. Analytical chemistry
  - d. Co-ordination chemistry
2. Recall the person who first developed ChemDraw in 1985.
  - a. Arhenius
  - b. Einstein
  - c. David A. Evans and Stewart Rubenstein
  - d. Betler
3. Pick out the tool used to split molecules across specific bonds
  - a. bond tool
  - b. eraser tool
  - c. atom tool
  - d. Mass Frag-mentation tool
4. Indicate the usage of Key 2 in bond hotkeys.
  - a. Used to change single bond in a given molecule
  - b. Used to change double bond in a given molecule
  - c. Used to change dashes line in a given molecule dashes line
  - d. Used to change triple bond in a given molecule
5. Locate the display data in Structure analysis window.
  - a. chemical formula
  - b. exact mass
  - c. molecular weight
  - d. All the above

6. How many Carbon atoms are present in Alanine?



- a.3
- b.2
- c. 1
- d.5

7. Recognise the usage of ALT+CTRL+N in Chemdraw.

- a. convert structure to name
- b. convert name to structure
- c. clean up structure
- d. delete atom in the molecule.

### **PART-B**

1. Compile the application of Hypercube and Gaussian molecular modelling software tools.
2. Illustrate the function of Shortcuts keys in Chemdraw.
3. Compute the function of Hotkeys in Chemdraw.
4. Outline the available advanced drawing techniques in Chemdraw.
5. Differentiate the chemdraw techniques on structural analysis and elemental analysis.

### **PART-C**

1. Outline the simulation techniques to create a TLC plate and display the  $R_f$  values.
2. Produce importing and exporting data in the chemdraw/Excel interface.
3. Summarize the various software tools available for molecular modelling with its application.
4. Predict the biomolecular drawing through software tool.
5. Employ the main tools palette to design chemical structure using chemdraw

## UNIT-5

# MODERN ENGINEERING MATERIALS FOR ELECTRONIC DEVICES

### **5.1. Introduction:**

An alloy is a homogeneous substance formed by mixing two or more elements, at least one of them being a metal. Most pure metals are either too soft, brittle or chemically reactive for practical use. Combining different ratios of metals as alloys modifies the properties of pure metals to produce desirable characteristics. The alloys made of aluminium, titanium, copper, and magnesium are also important metals. The magnetic alloy semiconductors containing lower concentrations of magnetic ions are known as dilute magnetic semiconductors. These alloys have recently attracted much attention because of their potential applications.

**Definition:** An alloy is a homogeneous substance formed by mixing two or more elements, at least one of them being a metal.

Alloys are of three types:

- 1) Alloys formed by two or more metals.  
Eg: brass (Cu-Zn)
- 2) Alloys formed between a metal and a non-metal
- 3) Alloys (Amalgam) formed between mercury and another metal

Eg: Zinc amalgam.

#### **5.1.1 Need for Alloys**

##### **1. To improve hardness**

Hardness of a metal is considerably increased on alloying it. Conversion of soft gold into hard gold by alloying it with copper is an example. The tensile strength of iron is increased ten times by alloying with 1% carbon.

##### **2. To lower the melting point**

It is lower for an alloy compared to the melting points of its constituents. e.g.; Melting point of solder ( $183^{\circ}\text{C}$ ) is less than those of its constituents; pb ( $327^{\circ}\text{C}$ ) and Sn ( $232^{\circ}\text{C}$ ). Alloying makes the metallic system easily fusible and so alloys can be moulded at lower temperatures compared to moulding temperatures of pure metal.

##### **3. To improve casting property**

Some metals expand on solidification. This arises due to requirement of formation of certain lattice arrangements of the metallic atoms as the metal solidifies. This property helps proper casting of metals into objects. Some solid metals are soft and brittle making their

castings weak. This deficient character is eliminated by alloying the metal. Molten alloys on solidification produce hard, durable castings. The alloy (pb + Sn + Sb) has excellent casting property when compared to its constituents.

#### **4. To modify the electrical conductivity**

Alloys are less conductive than pure metals. The interaction of two metals in an alloy modifies the electronic conduction bands in them to render the alloy less conductive. eg: even traces of metallic impurities in copper reduces its electrical conductivity.

#### **5. To modify the color**

Alloying modifies the colors of metals eg: red copper and silver – white zinc, on alloying, produces yellowish brown brass alloy.

#### **6. To modify chemical properties**

Chemical properties are either enhanced or depressed.eg: rate of dissolution of an alloy in hydrochloric acid is different (usuallyless) from the rates of dissolutions of the constituent metals. An alloy is less easily attacked by chlorine compounds than its constituent metals.

#### **7. To resist the corrosion of the metal**

The most important and useful property of alloying is its ability to resist corrosion in its alloying. Generally, alloys are more resistant to corrosion than pure metals. e.g.: stainless steel (alloy of Fe,C, Ni and Cr) which is not corroded by the atmospheric conditions though pure Fe easily corrodes (rusted) in moist air.

Of these property- modifications, enhanced fusion capability and resistant to corrosion are two qualities that make alloys very useful material industrially.

#### **5.2. Modern electronic grade alloys:**

Electronic grade alloys and electrical alloys have excellent mechanical properties, generally have high thermal and electrical conductivity, and are highly resistant to corrosion. These alloys are often used for electronic applications in anodes, lead wires, fuel cells, battery casings, packaging and lids.

##### **5.2.1 Nickel alloys:**

###### **Nickel 200**

###### **Composition:**

Ni-99.0% min, C-.15% max, Mn-.35% max, S-010% max, Si-.35% max, Cu-.25% max, Fe-.40%

###### **Properties:**

It is a commercially pure nickel that exhibits good corrosion resistance and has rather low electrical resistivity.

**Uses:**

It's used in caustic solutions, food handling equipment, and general corrosion-resistant parts and structures. Because it contains magnetic and mechanical properties, it can be used in devices that require magnetic actuated parts.

**Nickel 201**

**Composition:**

Ni- 99.0% min, C- 02% max, Mn-.35%, S-.010% max, Si-.35% max, Cu- .25% max, Fe-40%

**Properties:**

It is similar to Nickel 200 but low carbon content. It has a low annealed hardness and very low work-hardening rate.

**Uses:**

Desirable in deep drawing, spinning, and coining. In addition, it can be applied to corrosion-resistant equipment including but not limited to: caustic evaporators, spun anodes, and laboratory crucibles.

**Nickel 205**

**Composition:** Ni: >99%, Mn: <.35, Fe: <.20, Si: <0.15, Cu: 0.15, C: <0.15, Mg: 0.010-0.080, Ti : 0.010-0.050, S: <0.0080.

**Properties:**

It exhibits good oxidation resistance.

**Uses:**

It is frequently used in lead wires, pins, terminals, vacuum tube components, support wires, and comparable electrical parts.

**Nickel 270**

**Composition:**

It is a high purity nickel alloy

**Uses:**

It is commonly used for electrical resistant thermometers.

**Nichrome:**

It is an alloy of iron, nickel and chromium. Many types of nichrome alloys are possible based on the percentage of these metals-

**Composition:**

Ni-60%, Fe-26%, Cr-12%, Mn-25%

A steel alloyed with 10% nickel and 20% chromium can be used at  $100^{\circ}\text{C}$ . Steels containing 16 to 20% chromium with low carbon possess oxidation resistance up to  $900^{\circ}\text{C}$ . They are having high heat and chemical resistance.

**Uses:**

1. They are used in making furnace heating coils,
2. They are used in heating elements in electric irons, toasters and kettles,
3. They are used in gas turbines, aero engine valves, retorts, annealing boxes
4. They are used in equipment exposed to high temperatures and house hold appliances.

**Alnico:**

This is otherwise called by the name aluminium nickel-cobalt steel.

**Composition:**

Al- 10 to 12%, Ni-15 to 20%, Co- 40 to 60%

**Properties:**

It is highly magnetic and used as permanent magnets in motors.

**Uses:**

1. It is highly magnetic and used for making powerful magnets.
2. used as permanent magnets in motors generators, galvanometers etc.,

**5.2.2. Copper alloys:**

**Cupro nickel**

It is a part of the electronic grade alloy family. The earliest discovery of nickel copper was around 235 BC in Bactria. The original chemical breakdown was 75% copper and 25% nickel. Nickel copper is composed of elements such as iron and magnesium.

**Composition:**

10 % Cu/Ni, 88.6% Cu, 10 % Ni, 1.4 % Fe

**Properties:**

Nickel has a significant effect on the physical properties of the pairing. The color becomes lighter when nickel is added and the purity increases as well. It is among the corrosion resistant copper alloys, protecting against moisture, acids, alkalis and salt solutions, organic acids and gases such as oxygen, chlorine and carbon dioxide. The probability that Nickel copper will ever face corrosion is small due to the stable protective coating.

**Uses:**

1. It is often used in the marine industry due to its high electric resistance ability and corrosion while in sea water. It falls into the moderate to poor machining ability category due to its durability. This bond forms long, hard chips that cause irreparable surface damage when machined down.

2. It has been used in auto components, tools for marine exploration and in power plants; additionally, it is applied in coinage.

3. In electrical engineering space, where it can be used in the production of heating cables, anodes for TV tubes and electric resistors. This alloy can be easily worked while experiencing cold and hot temperatures.

4. This nickel copper alloy is used in electrical products, springs, bolts, diaphragms, and marine components.

#### **Copper 101 alloy:**

**Composition:** It is composed primarily of 99.90% pure copper with a trace amount of oxygen (.04%).

#### **Properties:**

It has excellent conductivity and malleability .In addition; it prevents corrosion and combines well with nickel, zinc, and aluminium. Copper can easily be recycled. Old pipes, taps, and car radiators made out of Copper can be melted down and reused without losing any properties. It has an excellent capacity for being both cold worked and hot formed.

#### **Uses:**

It is commonly used in the telecommunications industry and plays an important role in our economy. Being an electronic grade alloy, it's an excellent conductor of heat and electricity. Although it was once utilized in coins and even house décor, today it is more frequently used in roofing. It's also found in electronic conductors and glass to metal seals.

#### **Copper 102 alloy:**

**Composition:** It contains 99.95% copper and .05% oxygen

#### **Properties:**

It has an excellent capacity for being cold worked and hot formed. In addition, Copper 102 is durable and simple to combine (has high impact strength). It has low temperature properties and as its temperature decreases, its strength increases.

#### **Uses:**

It is also used in the telecommunications industry and has high electrical resistivity/conductivity. It has high ductility and high electrical and thermal conductivity. Vacuum tubes, electronic conductors, and glass to metal seals are a few examples of uses.

**Brass:**

This is the most important alloy of copper in which the percentage of zinc goes up to 45%. Besides zinc, a small number of other metals such as Sn, Mn, Al, Fe, Pb etc are also added to obtain special properties.

**Composition:**

Cu (60 – 90%), Zn (40 – 10%)

**Properties:**

These alloys possess greater strength, durability and machinability than copper. They have lower melting point than copper and zinc. They are corrosion resistant and water resistant.

**Uses:**

- 1) Ordinary brass is used for general utensils and general castings.
- 2) Muntz brass is used for hot stampings, sheets, hot rolled products, marine fillings, condenser tubes, radiator cores.
- 3) Leaded brass is used in making tubes, plates etc.,
- 4) High tensile brass is used in making switch gears, marine propeller shafts.
- 5) Naval brass is used for propellers and marine works
- 6) Aluminum bronze is used for condenser tubes in marine and other installation.
- 7) German silver is used for utensils, table wares, bolts, screws, imitation jewellery, cutlery decorative articles.

**5.2.3. Phosphorus alloys:****Phosphor bronze:****Composition:**

It is composed of copper, tin, and phosphorous. The addition of tin to this alloy, which is a part of the electronic grade family, makes it stronger and increases its ability to withstand corrosion; on the other hand, the addition of phosphorous makes the pairing stiffer.

**Properties:**

The physical properties of phosphor bronze include effective formability, solder ability, corrosion resistance, spring ability, and strength in general.

This copper-based alloy possesses an extreme freezing range, sufficient electrical conductivity, and low thermal conductivity.

**Uses:**

It has been used for many years in electrical components; some common applications include springs, sleeve bushings and bearings, welding rods, jewellery, guitar strings, dental bridges. It has many designer specifications and is a proven engineering material.

#### **5.2.4. Aluminium alloys:**

##### **Composition:**

In order to improve the capabilities of pure aluminium, particularly to increase its strength, other elements are added to the chemical composition. Iron, silicon, copper, magnesium, manganese, and zinc are some of the additional elements that can contribute up to 15% of the alloy's weight combined. Commercial electronic grade alloys are comprised of aluminum 99 percent or higher purity.

##### **Properties:**

They have excellent corrosion resistance, excellent workability, as well as high thermal and electrical conductivity.

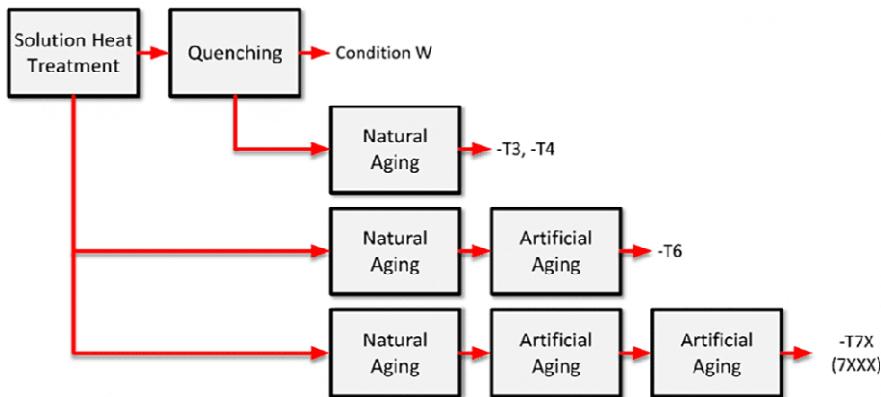
##### **Uses:**

It is commonly used for transmission, or power grid, lines that connect the national grids.

#### **5.2.4.1. Heat-Treatable Alloys**

Heat-treatable alloys are mixtures of metallic and non-metallic components consisting of pure aluminum that is heated up to a certain point, followed by the addition of alloying elements homogenously. The addition of the alloying material makes the aluminum become solid.

**Process:** Some alloys are strengthened by solution heat-treating and then quenching, or rapid cooling. Heat treating takes the solid, alloyed metal and heats it to a specific point. The alloy elements, called solute, are homogeneously distributed with the aluminium putting them in a solid solution. The metal is subsequently quenched, or rapidly cooled, which freezes the solute atoms in place. The solute atoms consequently combine into a finely distributed precipitate. This occurs at room temperature which is called natural aging or in a low temperature furnace operation which is called artificial aging.



**Figure 5.1. Flow chart for Heat-Treatable Alloys**

### 5.2.5. Silicon alloys:

Silicon alloys are a group of alloys that contain silicon as one of the primary components. They are widely used in various applications due to their unique combination of properties, including high strength, good corrosion resistance, excellent electrical conductivity, and high melting points. Some common silicon alloys include:

1. **Silicon-Manganese Alloy:** This alloy contains silicon and manganese, with silicon typically accounting for around 20-30% of the alloy composition. It is used in the production of stainless steel, as it improves the strength, ductility, and toughness of the steel.
2. **Silicon-Aluminum Alloy:** This alloy contains silicon and aluminum, with silicon typically accounting for around 5-40% of the alloy composition. It is used in the production of castings, as it improves the fluidity and cast ability of the molten metal, and also enhances the strength and ductility of the castings.
3. **Silicon-Copper Alloy:** This alloy contains silicon and copper, with silicon typically accounting for around 1-10% of the alloy composition. It is used in the production of electrical components, such as connectors and terminals, due to its excellent electrical conductivity and corrosion resistance.
4. **Silicon-Iron Alloy:** This alloy contains silicon and iron, with silicon typically accounting for around 1-3% of the alloy composition. It is used in the production of electrical steel, as it improves the magnetic properties and electrical resistivity of the steel.
5. **Silicon-Bronze Alloy:** This alloy contains silicon and bronze, with silicon typically accounting for around 1-3% of the alloy composition. It is used in the production of various components, such as marine hardware and electrical connectors, due to its high strength, good corrosion resistance, and excellent machinability.

Thus, silicon alloys are used in a wide range of applications due to their unique combination of properties. They are able to provide improvements in strength, ductility, castability, electrical conductivity, and magnetic properties, making them an important material choice for various industries. To properly control the quantum mechanical properties, the purity of the silicon must be very high. Bulk silicon wafers used at the beginning of the integrated circuit making process must first be refined to a purity of 99.999999% often referred to as "9N" for "9 nines", a process which requires repeated applications of refining technology. The use of silicon in semiconductor devices demand a much greater purity than afforded by metallurgical grade silicon. Very pure silicon (>99.9%) can be extracted directly from solid silica or other silicon compounds by molten salt electrolysis.

### **5.3. Application**

#### **5.3.1. Electrical components**

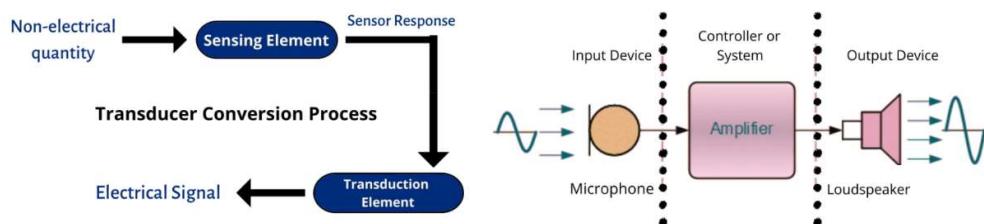
Alloys are widely used in electrical components due to their excellent electrical conductivity, mechanical strength, and resistance to corrosion. Some common applications of alloys in electrical components include:

1. **Copper Alloys:** Copper alloys such as brass and bronze are commonly used in electrical components due to their high electrical conductivity, excellent corrosion resistance, and good mechanical properties. They are used in electrical connectors, terminals, and conductors.
2. **Aluminum Alloys:** Aluminum alloys are also used in electrical components due to their good electrical conductivity, low density, and good thermal conductivity. They are commonly used in electrical conductors, busbars, and heatsinks.
3. **Silver Alloys:** Silver alloys are used in electrical components due to their excellent electrical conductivity, good mechanical properties, and resistance to oxidation. They are commonly used in electrical contacts, switches, and relays.
4. **Nickel Alloys:** Nickel alloys such as Monel and Inconel are used in electrical components due to their excellent corrosion resistance and high strength. They are commonly used in electrical connectors, terminals, and other components that require good corrosion resistance.
5. **Titanium Alloys:** Titanium alloys are used in electrical components due to their excellent strength-to-weight ratio and good corrosion resistance. They are commonly used in electrical conductors, connectors, and other components that require lightweight and high strength.

Thus, alloys play an important role in electrical components due to their ability to provide a wide range of mechanical, electrical, and corrosion-resistant properties. They are able to meet the demanding requirements of modern electrical systems, ensuring reliable and efficient performance.

### 5.3.2. Transducers:

An electrical device that transforms energy from one form to another is known as a transducer. It converts physical quantities into useful electrical signals or quantities such as electric current or voltage. For example, a temperature transducer converts temperature to equivalent electrical potential, sound into electricity or light into motion.



**Figure 5.2. Transducers**

Alloys are commonly used in transducers due to their excellent mechanical and electrical properties, such as high strength, good thermal stability, and excellent electrical conductivity. Transducers are devices that convert one form of energy into another, such as converting electrical signals into mechanical motion or vice versa. Some common applications of alloys in transducers include:

1. **Piezoelectric Alloys:** Piezoelectric alloys are used in transducers that convert mechanical motion into electrical signals or vice versa. These alloys generate electrical charges when subjected to mechanical stress or vibrations, making them useful in applications such as ultrasound imaging, pressure sensors, and vibration sensors.
2. **Nickel Alloys:** Nickel alloys such as Invar and Kovar are used in transducers that require high dimensional stability and resistance to thermal expansion. These alloys have low coefficients of thermal expansion, making them useful in applications such as temperature sensors, pressure sensors, and accelerometers.
3. **Titanium Alloys:** Titanium alloys are used in transducers that require high strength, good corrosion resistance, and good thermal stability. These alloys are useful in applications such as pressure sensors, flow meters, and vibration sensors.
4. **Copper Alloys:** Copper alloys such as brass and bronze are used in transducers that require high electrical conductivity and good thermal conductivity. These alloys are useful in applications such as strain gauges, pressure sensors, and temperature sensors.

Thus, alloys are an important material choice for transducers due to their ability to provide a wide range of mechanical, thermal, and electrical properties. They are able to meet the demanding requirements of modern transducer systems, ensuring accurate and reliable performance.

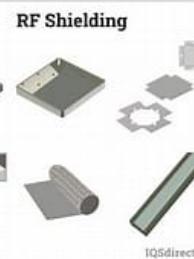
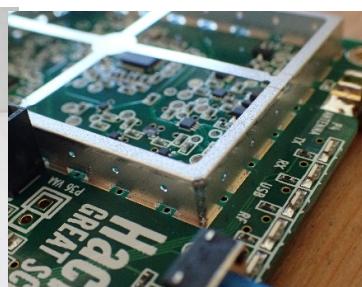
### 5.3.3. Electromagnetic shielding of computers:

Alloys are widely used in electromagnetic shielding of computers due to their excellent electrical conductivity and magnetic properties. Electromagnetic shielding is the process of creating a barrier around electronic devices to protect them from electromagnetic interference (EMI). EMI can cause disruption in electronic devices, leading to reduced performance or even damage.

Electromagnetic shielding is the practice of reducing the electromagnetic field in a space by blocking the field with barriers made of conductive or magnetic materials. Shielding is typically applied to enclosures to isolate electrical devices from the 'outside world', and to cables to isolate wires from the environment through which the cable runs. Electromagnetic shielding that blocks radio frequency electromagnetic radiation is also known as radio frequency (RF) shielding.



Figure. 5.3.a.Electromagnetic shielding



RF Shielding

Some common alloys used in electromagnetic shielding of computers include:

1. **Copper Alloys:** Copper alloys such as brass and bronze are commonly used in electromagnetic shielding of computers due to their excellent electrical conductivity and good magnetic properties. They are used in components such as shielding tapes, gaskets, and braids.

2. **Nickel Alloys:** Nickel alloys such as Mu-metal and Permalloy are used in electromagnetic shielding of computers due to their high magnetic permeability, which makes them effective in shielding against magnetic fields. They are used in components such as magnetic shields and transformer cores.

3. **Steel Alloys:** Steel alloys such as carbon steel and stainless steel are used in electromagnetic shielding of computers due to their good magnetic properties and high

mechanical strength. They are used in components such as shielding plates, cabinets, and enclosures.

4. **Aluminum Alloys:** Aluminum alloys are used in electromagnetic shielding of computers due to their good electrical conductivity and lightweight properties. They are used in components such as shielding foils and tapes.

Thus, alloys are an important material choice for electromagnetic shielding of computers due to their ability to provide a wide range of electrical, magnetic, and mechanical properties. They are able to meet the demanding requirements of modern electronic systems, ensuring reliable and efficient performance

#### **5.3.4. Telecommunication equipment:**

Alloys are widely used in telecommunication equipment due to their excellent mechanical, electrical, and thermal properties. Some of the common applications of alloys in telecommunication equipment include:

1. **Copper Alloys:** Copper alloys such as brass and bronze are commonly used in telecommunication equipment due to their excellent electrical conductivity and resistance to corrosion. They are used in connectors, cables, and other components that require high conductivity.

2. **Aluminum Alloys:** Aluminum alloys are also used in telecommunication equipment due to their low density, high strength-to-weight ratio, and good thermal conductivity. They are commonly used in antennas, reflectors, and other components that require lightweight and good thermal management.

3. **Stainless Steel Alloys:** Stainless steel alloys are used in telecommunication equipment due to their high strength, good corrosion resistance, and good thermal stability. They are used in enclosures, support structures, and other components that require durability and protection against harsh environments.

4. **Nickel Alloys:** Nickel alloys such as Invar are used in telecommunication equipment due to their low coefficient of thermal expansion and high dimensional stability. They are commonly used in components that require high precision and stability, such as waveguides and resonators.

so, alloys are an important material choice for telecommunication equipment due to their ability to provide a wide range of mechanical, electrical, and thermal properties. They are able to meet the demanding requirements of modern telecommunication systems, ensuring reliable and efficient communication

#### **5.3.5. Rocket motor casings:**



**Figure 5.4a**Rocket motor case



**Figure. 5.4b**Powder metallurgy products

Rocket motor casings are subjected to high temperatures, pressures, and stresses during the operation of a rocket. Therefore, materials with high strength, good corrosion resistance, and good thermal stability are required for rocket motor casings. Alloys are commonly used in rocket motor casings due to their excellent mechanical and chemical properties.

Some of the common alloys used in rocket motor casings include:

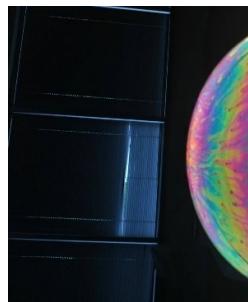
1. **Aluminum Alloys:** Aluminum alloys are commonly used in rocket motor casings due to their low density, high strength-to-weight ratio, good corrosion resistance, and good thermal stability. They are also relatively inexpensive, making them a cost-effective option.
2. **Titanium Alloys:** Titanium alloys are another popular choice for rocket motor casings due to their excellent strength-to-weight ratio, good corrosion resistance, and good thermal stability. They can also withstand high temperatures, making them suitable for use in rocket motor casings.
3. **Inconel Alloys:** Inconel alloys are a family of nickel-chromium-based super alloys that are known for their excellent high-temperature strength and resistance to corrosion and oxidation. They are commonly used in rocket motor casings due to their ability to withstand high temperatures and corrosive environments.
4. **Steel Alloys:** Steel alloys are also used in rocket motor casings due to their high strength, good thermal stability, and good resistance to corrosion. They are particularly useful in applications where high strength is required.

Therefore, alloys are an important material choice for rocket motor casings due to their excellent mechanical, thermal, and chemical properties. They are able to withstand the extreme conditions encountered during rocket motor operation, ensuring the safety and reliability of the rocket.

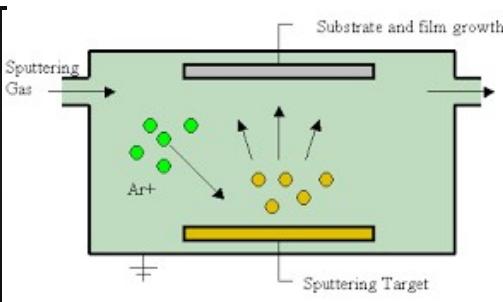
#### **5.4. Thin film**

A thin film is a layer of material ranging from fractions of a nanometer (monolayer) to several micrometers in thickness. The controlled synthesis of materials as thin films (a process referred to as deposition) is a fundamental step in many applications.

A familiar example is the household mirror, which typically has a thin metal coating on the back of a sheet of glass to form a reflective interface. The process of silvering was once commonly used to produce mirrors, while more recently the metal layer is deposited using techniques such as sputtering.



**Figure. 5.5a Thin film optics**



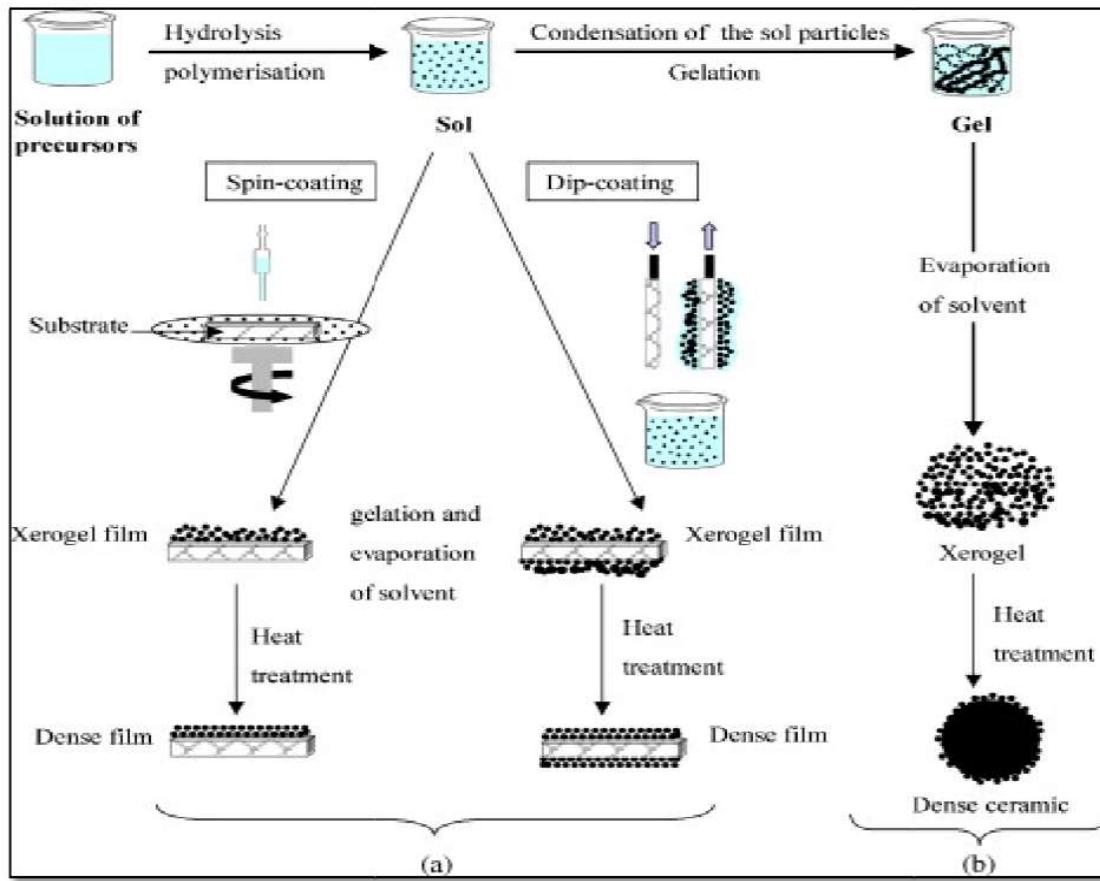
**Figure. 5.5b Sputtering deposition**

Advances in thin film deposition techniques during the 20th century have enabled a wide range of technological breakthroughs in areas such as magnetic recording media, electronic semiconductor devices, LEDs, optical coatings (such as antireflective coatings), hard coatings on cutting tools, and for both energy generation (e.g. thin film solar cells) and storage (thin-film batteries). It is also being applied to pharmaceuticals, via thin-film drug delivery.

In addition to their applied interest, thin films play an important role in the development and study of materials with new and unique properties. It includes multiferroic materials, and super lattices that allow the study of quantum confinement by creating two-dimensional electron states.

#### 5.4.1. Preparation by the Sol-Gel Method

- (i) The sol-gel process is a technique used in materials science to produce solid materials from small molecules.
- (ii) It is used for the fabrication of metal oxides, especially the oxides of silicon and titanium.
- (iii) It involves conversion of monomers into a colloidal solution (*sol*) that acts as the precursor for an integrated network (*gel*) of either discrete particles or network polymers.
- (iv) Typical precursors are metal alkoxides.



**Figure. 5.6. Steps for preparation of thin films and powder by Sol-gel process**

#### 5.4.1.1. Stages in the process

In this chemical procedure, the 'sol' (or solution) gradually evolves towards the formation of a gel-like diphasic system containing both a liquid phase and solid phase whose morphologies range from discrete particles to continuous polymer networks. In the case of the colloid, the volume fraction of particles (or particle density) may be so low that a significant amount of fluid may need to be removed initially for the gel-like properties to be recognized. This can be accomplished in any number of ways. The simplest method is to allow time for sedimentation to occur, and then pour off the remaining liquid. Centrifugation can also be used to accelerate the process of phase separation.

#### Drying process

Removal of the remaining liquid (solvent) phase requires a drying process, which is typically accompanied by a significant amount of shrinkage and densification. The rate at which the solvent can be removed is ultimately determined by the distribution of porosity in the gel. The ultimate microstructure of the final component will clearly be strongly influenced by changes imposed upon the structural template during this phase of processing.

### **Thermal treatment, or firing process**

In order to favour further polycondensation and enhance mechanical properties and structural stability via final sintering, densification and grain growth. One of the distinct advantages of using this methodology as opposed to the more traditional processing techniques is that densification is often achieved at a much lower temperature.

The precursor sol can be either deposited on a substrate to form a film (e.g., by dip coating or spin coating), cast into a suitable container with the desired shape (e.g., to obtain monolithic ceramics, glasses, fibers, membranes, aerogels), or used to synthesize powders (e.g., microspheres, nanospheres).

### **Advantage of Sol-gel process**

The sol-gel approach is a cheap and low-temperature technique that allows for the fine control of the product's chemical composition. Even small quantities of dopants, such as organic dyes and rare earth elements, can be introduced in the sol and end up uniformly dispersed in the final product. It can be used in ceramics processing and manufacturing as an investment casting material, or as a means of producing very thin films of metal oxides for various purposes.

Sol-gel derived materials have diverse applications in optics, electronics, energy, space, (bio)sensors, medicine (e.g., controlled drug release), reactive material and separation (e.g., chromatography) technology.

#### **5.4.2. Applications of thin films**

Thin films are thin layers of material, typically ranging in thickness from a few nanometers to several micrometers. They are used in a wide range of applications in various fields, such as electronics, optics, solar cells, coatings, and biomedical applications.

The controlled synthesis of materials as thin films is a fundamental step in many applications. Thin films can be produced through a variety of deposition techniques, such as chemical vapor deposition, sputtering, and evaporation. In these techniques, atoms or molecules are deposited onto a substrate surface, where they form a thin film. The properties of the thin film, such as its thickness, composition, and structure, can be controlled by adjusting the deposition conditions, such as the temperature, pressure, and gas composition.

Thin films can have unique properties that differ from their bulk counterparts. For example, a thin film of a material may exhibit different electronic or optical properties than the same material in bulk form. This is due to the quantum confinement effect, where the thickness of the thin film is comparable to the size of the material's electronic wave function.

1. **Electronics and Optoelectronics:** Thin films find extensive use in electronics and optoelectronics industries. They are used in the production of microelectronic devices, such as transistors, diodes, capacitors, and resistors. These devices are made by depositing thin films of materials such as silicon, copper, and aluminum onto a substrate such as glass or silicon.

Thin film deposition techniques such as chemical vapor deposition (CVD) and physical vapor deposition (PVD) are used to make these devices. Thin films are also used to make various types of sensors, including gas sensors, biosensors, and chemical sensors. In optoelectronics, thin films are used to make thin-film solar cells, LED displays, and OLEDs (organic light-emitting diodes).

2. **Optics:** Thin films are used in optics to create interference filters, anti-reflection coatings, and mirrors. These films are made by depositing layers of materials with different refractive indices onto a substrate. The thickness and composition of these layers can be precisely controlled to create the desired optical properties.

3. **Coatings:** Thin films are used in coatings to provide corrosion resistance, wear resistance, and other properties to surfaces. These films can be deposited onto a wide range of materials such as metals, ceramics, and polymers. For example, thin-film coatings are used in the aerospace industry to protect aircraft surfaces from corrosion and wear. They are also used in the automotive industry to improve the durability and scratch resistance of automotive parts.

4. **Optical Coatings:** Thin films are widely used as optical coatings in the production of mirrors, lenses, and other optical components. These coatings can be designed to reflect or transmit specific wavelengths of light.

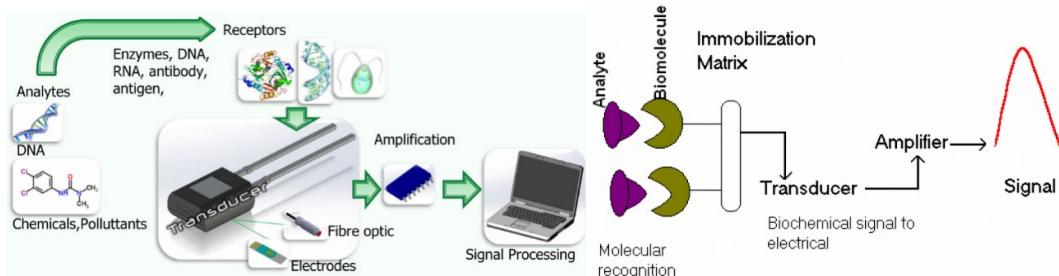
5. **Magnetic Storage:** Thin films are used in the production of magnetic storage media such as hard disk drives, floppy disks, and magnetic tapes. Magnetic thin films are also used in the production of MRAM (magnetic random access memory), a type of non-volatile memory that can be used in electronic devices.

6. **Solar cells:** Thin films are used in solar cells to convert sunlight into electricity. Thin film solar cells are made by depositing layers of materials such as cadmium telluride, copper indium gallium selenide, or amorphous silicon onto a substrate. These cells are lightweight and flexible and can be made into large sheets that can be easily installed on rooftops or other structures.

7. **Photovoltaic Cells:** Thin films are widely used in the production of photovoltaic cells or solar cells. These cells are made from semiconductor materials like silicon, cadmium

telluride, copper indium gallium selenide, and others. Thin-film solar cells are lighter, more flexible, and less expensive to produce than traditional solar cells.

8. **Biomedical applications:** Thin films are used in biomedical applications such as drug delivery, tissue engineering, and biosensors. These films can be made from biocompatible materials such as polymers, ceramics, and metals. Thin film deposition techniques such as electrospinning, spin coating, and layer-by-layer assembly are used to make these films. They can be used as coatings for medical devices like stents and implants to improve their biocompatibility and reduce inflammation. Thin films are also used to make biosensors for detecting glucose, cholesterol, and other biomolecules.



**Figure. 5.7. Biosensor materials for advanced research and technology**

In conclusion, thin films are versatile materials that are used in a wide range of fields. They are used to make microelectronic devices, optical components, solar cells, coatings, and biomedical devices. The properties of thin films can be precisely controlled, making them ideal for many applications.

### **Part A**

1. Analyze the correct statement regarding the melting point of alloys.
  - a) The melting point of alloys is always higher than the melting points of its constituents.
  - b) The melting point of alloys is always lower than the melting points of its constituents.
  - c) The melting point of alloys can be either higher or lower than the melting points of its constituents.
  - d) Alloying has no effect on the melting point of metallic systems.
2. Recognize the common use of Nickel 200.
  - a) Food handling equipment
  - b) Structural parts
  - c) Devices requiring magnetic actuated parts
  - d) All of the above
3. Identify Alnico
  - a) A type of aluminum alloy
  - b) A type of nickel alloy
  - c) A type of cobalt alloy
  - d) A type of aluminum nickel-cobalt steel
4. Select cupro nickel from the given combination.
  - a) An alloy of copper and nickel with iron and magnesium
  - b) An alloy of copper and zinc with nickel
  - c) An alloy of copper, tin, and phosphorus
  - d) An alloy of copper and tin with phosphorus
5. Match any one of the following with the property of brass.
  - a) Low machinability
  - b) High melting point
  - c) Water resistance
  - d) Low durability
6. Choose which one is a transducer
  - a) A device that stores electrical energy
  - b) A device that converts electrical energy into mechanical energy
  - c) A device that transforms energy from one form to another
  - d) A device that measures the intensity of an electrical signal
7. Recall common application of thin films
  - a) Household insulation
  - b)Food packaging
  - c)Reflective coatings
  - d)Structural materials

### **PART B**

1. State the importance of electronic grade alloys with suitable examples.
2. Discuss heat-treatable alloys using a flowchart.
3. Describe how alloys are incorporated into telecommunication devices.
4. Interpret the significance of alloys for transducers.
5. Identify the role that alloys perform in the rocket motor casings.

### **PART C**

1. Analyze a detailed description of the composition, properties, and uses of nickel alloys.
2. Explain the composition, properties, and uses of copper alloys.
3. Recognize the use of alloys composed of silicon and aluminium in electrical and electronic components.
4. Define thin film and describe the sol-gel technique used to produce thin films.
5. Relate the various applications for thin film in each field.



**Semester Vara Pothu Padida..!**

